

IDC DOCUMENTATION

IDC Processing of Radionuclide Data

Notice

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About this Document

This section describes the organization and content of the document and includes the following sections:

- Purpose
- Scope
- Audience
- Related Information
- Using This Document

PURPOSE

This document is Revision 2 of *IDC Processing of Radionuclide Data User Guide*, first published March 1999 as [IDC5.2.2]. The following changes have been made to this publication.

- ## SCOPE

December 2001 IDC-5.2.2R2

AUDIENCE

This document is intended for scientists, technicians, and managers involved in the operation, maintenance, and/or use of the IDC and the data products that it provides.

RELATED INFORMATION

Use this document in conjunction with the following:

- *Analyst Instructions for Radionuclide Data* [IDC6.2.6Rev2]
- *Radionuclide Software User Manual* [IDC6.5.10Rev2]
- *Radionuclide Software Design* [IDC7.1.10Rev2]

See “References” on page 82 for a listing of all the sources of information consulted in preparing this document.

USING THIS DOCUMENT

This document is organized as follows:

- Overview
This chapter is a high-level overview of the collection of radionuclide sample data and the sequence of processing at the IDC for radionuclide data.
- Automatic Processing
This chapter describes the automatic processing performed on sample data immediately upon receipt at the IDC.
- Interactive Analysis
This chapter describes processing performed by the interactive review tools.
- Post-analysis Processing
This chapter describes the processing performed on the data after interactive analysis.
- References
This section lists the sources cited in this document.

■ Glossary

This section defines the terms, abbreviations, and acronyms used in this document.

Conventions

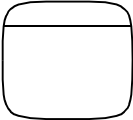
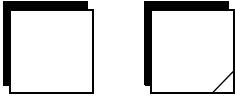

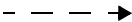
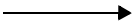
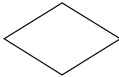

This document uses a variety of conventions, which are described in the following tables. [Table I](#) shows the typographical conventions.

TABLE I: TYPOGRAPHICAL CONVENTIONS

Element	Font	Example
database table	bold	dataready
database table and attribute when written in the dot notation		prodtrack.status
attributes of database tables when written separately	<i>italics</i>	<i>status</i>
processes and software units		<i>ParseSubs</i>
user-defined arguments		delete-remarksobject
computer code and output	courier	>(list 'a 'b 'c)
filenames, directories, and websites		amp.par
text that should be typed in exactly as shown		edit-filter-dialog

Table II shows the conventions for data flow diagrams.

TABLE II: DATA FLOW SYMBOLS

Description	Symbol
process	
external source or sink of data (left)	
duplicated external source or sink of data (right)	
data store (left)	
duplicated data store (right)	
control flow	
data flow	
decision	
product	

▼ About this Document

Chapter 1: Overview

This chapter provides a high-level overview of how the IDC processes radionuclide data and includes the following sections:

- Sample Collection
- Sample Processing
- Data Analysis

Chapter 1: Overview

The objective of radionuclide processing is to analyze International Monitoring System (IMS) radionuclide data and produce standard radionuclide products according to the *IDC Operations Manual* [CTB00a]. The automatic processing also serves to aid in monitoring the state-of-health (SOH) of a station and its associated detector.

To achieve these objectives, all radionuclide data received from operating IMS stations must be successfully processed. There are several types of IMS radionuclide data: pulse height data (PHD), meteorological (MET) data, SOH data, alert data, and data from certified radionuclide laboratories. Only PHD types (e.g., BLANKPHD, CALIBPHD, DETBKPHD, GASBKPHD, QCPHD, and SAMPLEPHD) are automatically analyzed. The processing for the other data types is restricted mainly to import and export. Because of this, the emphasis of this document is primarily on the processing of radionuclide PHD.

SAMPLE COLLECTION

Radionuclide stations sample the atmosphere in time intervals of 24 hours or less with the objective of detecting traces of radioactive gases and aerosols that may have originated from a nuclear weapons test. The time frame in which a station might pick up traces of fission products depends on the distance from the station to the event, as well as local and global weather patterns. Wind speed, wind direction, precipitation, and temperature gradients strongly affect the time of detection and signature intensity. It can take from several hours up to approximately two weeks for a radionuclide station to detect radioactive effluents, if a detection is made at all.

SAMPLE PROCESSING

Particulate stations are required to report sample data to the IDC within 72 hours after the commencement of sample collection. During this time period, particulate samples are allowed a substantial decay time and then counted on a High-Purity Germanium (HPGe) detector for at least 20 hours.

Noble gas stations have different requirements for processing times. These stations are required to report sample data to the IDC within 48 hours after the commencement of sample collection. Noble gas samples are chemically processed after sample collection and then counted for a maximum of 24 hours. Acceptable measurement modes for noble gas samples include high resolution gamma (γ) spectroscopy and beta-gamma (β - γ) coincidence. Chemical processing entails passing the noble gas sample through various traps and sieves to separate xenon (Xe) from other atmospheric gases that can interfere with the detection of radiation emitted by the radionuclides.

DATA ANALYSIS

There are three major processes that are usually performed at least once on most PHD types: automatic processing, interactive review, and post-analysis processing (Figure 1). Each sample data set is automatically processed using techniques that are specific to the detection mode: currently, *rms_xanalyze* is used to analyze 3-D β - γ coincidence data while *rms_analyze* is used to analyze all other data types.

The goals of automatic processing of PHD are:

- analyze the signatures of radionuclides in the data and extract parameters that can be used to quantify activity concentrations;
- prioritize the sample based on the results of the radionuclide analysis according to the probability that the sample contents are not from natural sources;
- monitor the SOH of a station and the detector on which samples are counted.

The results of the automated analysis are provided immediately after processing in the Automated Radionuclide Report (ARR).

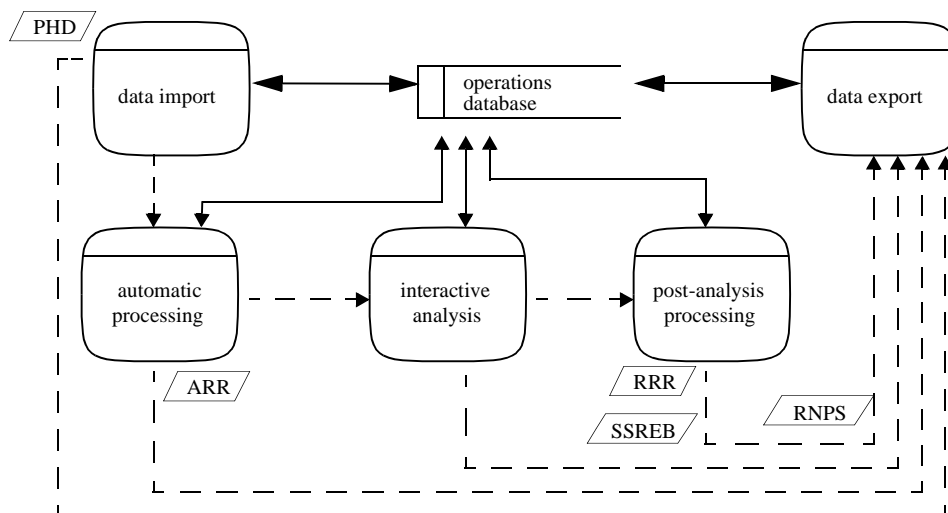


FIGURE 1. SYSTEM FUNCTIONAL MODEL

Interactive analysis is performed by a team of experts who review the automated results of a sample. They check for many things including

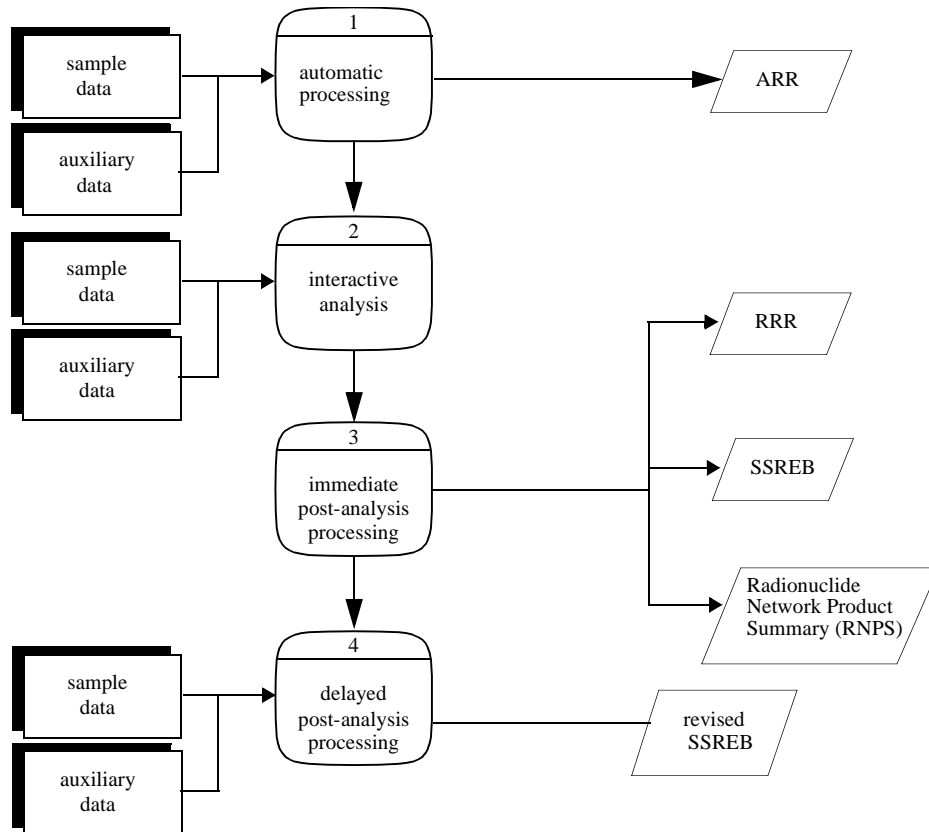
- false detections (Type I errors),
- radionuclide signatures that might have been missed by the automated processing (Type II errors), and
- data quality.

Comments are added to a sample when errors in the automated results are found. Sample data may be reanalyzed and/or reprioritized during this step in the radionuclide data processing. Upon release, a category level is assigned to a sample by the analyst to indicate the probability that the radionuclides detected in the sample are not of natural origin. Analysts use data such as meteorological data and SOH information to check for data quality.

When interactive analysis is complete, post-analysis processing is applied to the data. Post-analysis processing automatically compiles sample characteristics and event screening results into the Reviewed Radionuclide Report (RRR) and Standard Screened Radionuclide Event Bulletin (SSREB).

Each of these major data processing functions uses the operations database to store and access sample information. Sample data are available to personnel through access to the ORACLE database tables. Access is achievable via SQL queries, PL/SQL programs, Trendvue, the Data Workbench, Inspectra and CORIANT.

The sequence for IDC processing of radionuclide data, with time increasing downward, is shown in [Figure 2](#).

**FIGURE 2. RADIONUCLIDE DATA PROCESSING FLOW**

Chapter 2: Automatic Processing

This chapter describes how data from radionuclide IMS stations is automatically processed and includes the following sections:

- Overview
- Data Import
- Analysis of Gamma Spectrometry Data
- Analysis of 3-D Beta-Gamma Coincidence Data
- Quality Control Tests
- Prioritization
- Database Flags
- Creating Automated Radionuclide Reports

Chapter 2: Automatic Processing

OVERVIEW

The tasks of automatic processing of IMS radionuclide data include

- data import
- analysis
- quality control testing
- sample prioritization
- database flags
- notification of subscribers of high priority samples
- ARR production.

Data import involves checking data quality, parsing and storing properly formatted data, and notifying subscribers of alert (ALERT) messages and changes in detector calibrations. Details of these processes can be found in [IDC7.1.10Rev1]. Analysis includes radionuclide identification, quantification, and calculation of minimum detectable concentrations (MDCs). Depending on the detection mode, PHD are analyzed at the IDC with different codes. If PHD are from a site employing 3-D β - γ coincidence detection, then data are analyzed with *rms_xanalyze*. If PHD are from a site employing γ -spectrometry or 2-D β - γ coincidence detection, then data are analyzed with *rms_analyze*. Both analysis algorithms are described in this chapter. Descriptive information about errors that occur during processing is written to log files.

The detailed steps for automatic processing of radionuclide data are shown in [Figure 3](#). These are described in the sections that follow. (Steps 3 and 5 are not performed for 3-D β - γ coincidence data.)

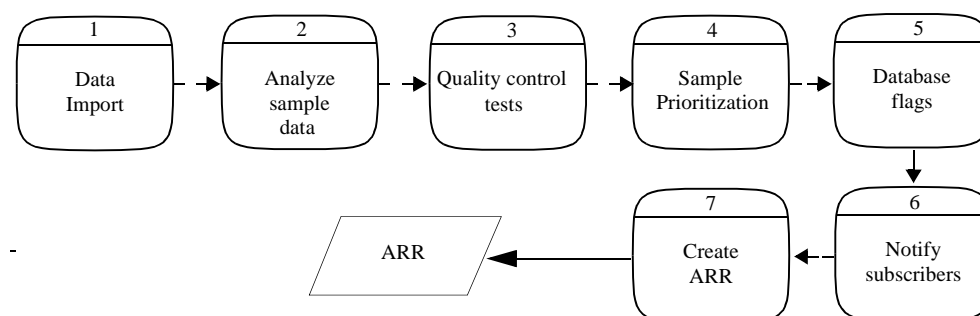


FIGURE 3. AUTOMATIC PROCESSING OF RADIONUCLIDE DATA

DATA IMPORT

The detailed steps of radionuclide data import are illustrated in [Figure 4](#) below.

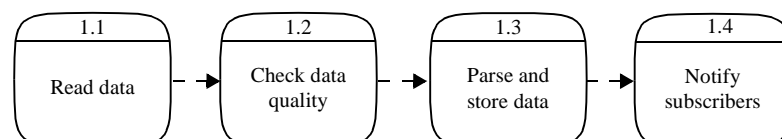


FIGURE 4. AUTOMATIC IMPORT OF RADIONUCLIDE DATA

Prior to processing, the data are read, checked for quality, and stored. Radionuclide data types that are not recognized by the processing system or are discontinued data types are saved in `$RMS_HOME/data/other`. Acceptable radionuclide data types that are not properly formatted are saved in `$RMS_HOME/data/new`.

The data quality tests performed on PHD include a check that the `#g_Spectrum` block contains only numerical data as well as a verification that the total air volume sampled in the `#Header` block is within 10% of that derived from the volume of elemental Xe in the sample. For the latter test, the following relation is used to determine the amount of expected air volume sampled.

$$V_{\text{air}} = \frac{V_{\text{Xe}}}{0.087}$$

where V_{air} is in m^3 and V_{xe} is in cm^3 .

This is by no means the only quality tests performed on the data. Most of the tests consider the quality of the data formats.

If the data type is acceptable and the message is properly formatted, the radionuclide data message may be assigned an identification (ID) number depending on the data type: PHD messages (such as SAMPLEPHD, GASBKPHD, DETBKPHD, CALIBPHD, QCPhD, and BLANKPHD) are assigned sample IDs, Radionuclide Laboratory Reports (RLRs) are assigned RLR IDs, and Radionuclide Monitoring System State of Health (RMSSOH) messages are assigned SOH IDs. All acceptable data types that are properly formatted are parsed and stored in the database tables, and the original messages are saved as flat files in `$RMS_HOME/data/processed`. PHD and RLRs without the mail headers are also stored in appropriately named folders located in `$RMS_HOME/data`. Subscribers are notified of ALERT messages and changes in detector calibrations.

ANALYSIS OF GAMMA SPECTROMETRY DATA

This section describes the analysis algorithm applied to radionuclide PHD from sites employing high resolution, low-resolution, or β -gated γ -spectrometry. (The last two γ -spectrometry data types are acquired by the ARIX noble gas system.) The analysis program is called *rms_analyze* and its processing steps are illustrated in [Figure 5](#) below. This section will focus on processes 2.1 through 2.9.

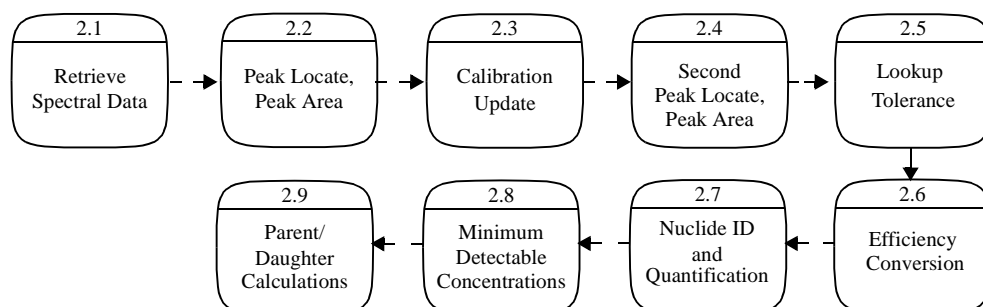


FIGURE 5. AUTOMATIC PROCESSING OF HIGH RESOLUTION γ -SPECTROMETRY DATA

Several of the automatic processing steps in *rms_analyze* are performed using Commercial Off The Shelf (COTS) software from Canberra Industries. Those that are dependent upon Canberra's Genie-2000 Spectroscopy Tools software [Can97] include the following:

- Process 2.2: Peak Locate, Peak Area
- Process 2.4: Second Peak Locate, Peak Area
- Process 2.7: Nuclide ID and Quantification
- Process 2.8: Minimum Detectable Concentrations.

Retrieve Spectral Data

This function retrieves sample, spectrum, energy, efficiency, resolution, and processing data from the UNIX file system, the ORACLE database, and the command line. These data are used to build a binary `.cnf` file in a proprietary Canberra format on the UNIX file system for use in subsequent analyses [IDC7.1.10Rev1]. Data are both read and written to this file during automatic analysis.

Peak Locate, Peak Area

Peak location and area determination are achieved via the Genie-2000 Spectroscopy Tools software. This COTS product is included with the IDC radionuclide processing software package. Included here is a summary of the peak location and peak area determination algorithms used by Genie-2000. A more technical discussion of these processes can be found in [Can97].

Peak Locate

The main input to the peak locate function is the `.cnf` file created during data retrieval (see “[Retrieve Spectral Data](#)” above). The energy range of the peak search is defined by the parameters `peak_start` and `peak_end`. Both can be found in `gards_proc_params_template` and are expressed in keV. The processing converts `peak_start` and `peak_end` from energy units into channel units. This is done by using the inversion of the linear part of the energy vs. channel regression (ECR) equation.

The ECR is a polynomial reconstituted from coefficients stored in `gards_energy_cal`. It has the general form:

$$E(c) = \sum_{i=0}^a \xi_i \cdot c^i$$

where E is energy in keV, c is the spectrum channel number, a is a number between 1 and 3, and ξ_i is the coefficient set. When `peak_start` and `peak_end` are converted, the inversion of the truncated linear ECR is used:

$$c(E) = \frac{(E - \xi_0)}{\xi_1}$$

Nominally, the coefficients from the most recent prior sample (MRP) counted on the same detector are retrieved and initially written to `gards_energy_cal`. Alternately, default energy coefficients can be retrieved from the database or entered at the command line and written to `gards_energy_cal`. As another alternative, an ECR based on the energy/channel data transmitted with the sample spectrum in the `#g_Energy` block can

be used instead. (These energy/channel pairs originate from the last detector calibration.) The ECR coefficients determined from the last detector calibration are automatically calculated and stored in **gards_energy_cal_orig**.

Once *peak_start* and *peak_end* are converted to channels, the Genie-2000 software attempts to locate peaks via a finite-impulse-response (FIR) digital filtering technique: the Generalized Second Difference Method [Can97]. In this technique, a filter with a Gaussian shape and net area of zero is convolved with the spectral data and passed across the spectrum from low to high energies. The initial ECR and resolution vs. energy regression (RER) equations are both required for determining the expected peak widths used in the filter.

The RER is reconstituted from the coefficients in **gards_resolution_cal** and has the general form below:

$$\text{FWHM}(E) = \alpha_0 + \alpha_1 \sqrt{E}$$

where FWHM is the peak width in keV at half the maximum peak height, E is energy in keV, and α_0 and α_1 comprise the coefficient set. Like the ECR, the coefficients from the MRP are used as the default values. However, RER coefficients can be entered at the command line and thus written to **gards_resolution_cal**. If the RER does not represent the current state of the instrument, that is, the actual peaks are wider or more narrow than that predicted by the RER, then the peak location function will fail to provide acceptable results.

The expected peak widths are used to determine a set of filter coefficients for each spectrum channel; these coefficients represent the zero net-area Gaussian peak. The number of coefficients required for each channel may vary, the number being dependent upon the coefficient values.

The processing finds the convolution of the zero net-area Gaussian shape with the pulse height data at every channel, and weights the result according to its standard deviation. (See [Can97] for the mathematical details of this procedure.) If the output of this operation is negative and its absolute value (i.e., the peak search sensitivity) exceeds the user-

defined multiple (`gards_proc_params_template.peak_sense`) of the standard deviation (i.e., the peak search sensitivity threshold), a peak region is defined. The centroid of the peak region is then determined.

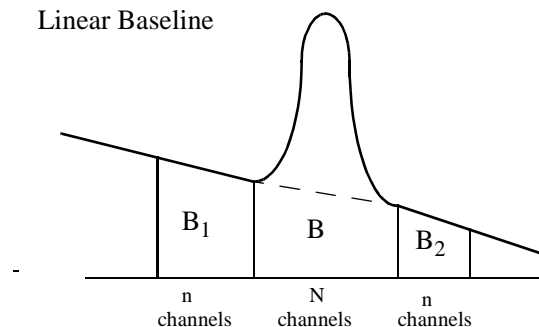
Once the filtering operation has produced a list of candidate peaks, additional calculations are performed to define a region-of-interest (ROI) about each centroid. Limits are placed on the width of the ROIs based on the expected FWHM for the peak at the centroid energy. The parameters, `gards_proc_params_template.left_fwhm_lim` and `right_fwhm_lim`, are both multiples of the RER-predicted FWHM.

An additional test is performed to determine if a peak region is comprised of multiple photon lines. The expected FWHM (`gards_proc_params_template.fwhm_mult_width`) is also used in this procedure.

Peak Area

At this time, the continuum (baseline) under the identified peaks is defined. There are two types of baseline models available (`gards_proc_params_template.back_type`): linear and step. In both instances, counts from a number of channels, n , on either side of the ROI (`gards_proc_params_template.back_chan`) are used for the baseline (B) determination (Figure 6).

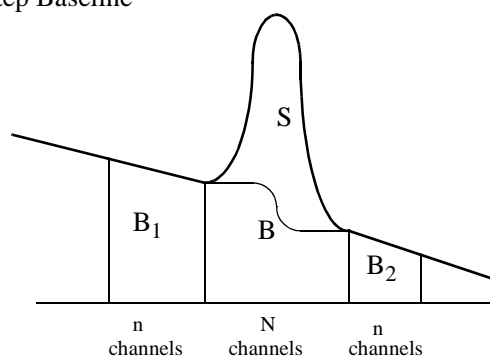
Linear Baseline



$$B = \left(\frac{N}{2n}\right)(B_1 + B_2)$$

$$\sigma_B = \left(\frac{N}{2n}\right)\sqrt{(B_1 + B_2)}$$

Step Baseline



$$B = \sum_{i=1}^N \left(\frac{B_1}{n} + \frac{(B_2 - B_1)}{n(S + B)} \sum_{j=1}^i y_j \right)$$

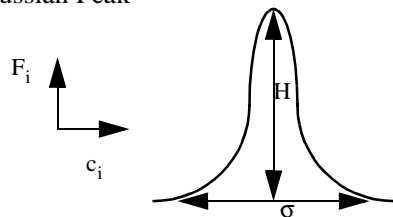
FIGURE 6. BASELINE CALCULATION

Once the ROIs have been defined and the net counts calculated (net = gross - baseline), the peak areas are estimated. The peak area determination is different for singlet vs. multiplet peaks. For singlets, there are several methods (`gards_proc_params_template.fit_singlets`) available for calculating the peak area. These include:

- summing the net counts in the ROI
- fitting the data with a Gaussian model using the least squares method
- fitting the data with a modified Gaussian shape (includes tailing effects)

See [Figure 7](#).

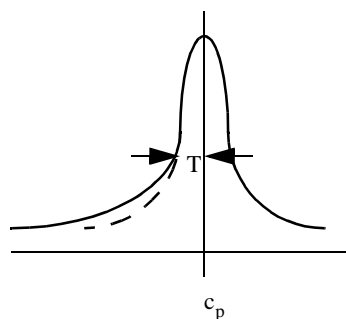
Pure Gaussian Peak



$$F_i = H \cdot e^{-\frac{(c_i - c_p)^2}{2\sigma^2}}$$

$$\sigma = 2.355 \cdot \text{FWHM}$$

Modified Gaussian Peak



$$F_i = \begin{cases} H \cdot e^{-\frac{(c_i - c_p)^2}{2\sigma^2}}, & c_i > c_p - T \\ H \cdot e^{-\frac{T(2c_i - 2c_p + T)}{2\sigma^2}}, & c_i < c_p - T \end{cases}$$

FIGURE 7. GAUSSIAN PEAK-FITTING MODELS

At present, only the unmodified Gaussian model is used for determining singlet peak areas. The following options are available for this type of peak fit:

- fix the peak widths at the value predicted by the RER (`gards_proc_params_template.fix_fwhm=1`), or
- leave the peak width as a free parameter to be estimated (`fix_fwhm=0`).

To determine the peak areas within multiplets, the ROI is deconvolved by assuming the multiplet peaks have a perfect Gaussian shape.

If the parameter `gards_proc_params_template.crit_level` is set to “1,” the estimated net areas are subject to a simple Critical Level Test (CLT). This is a type of signal-to-noise test. The CLT checks that the estimated net peak area is above a multiple of the variability of the ROI baseline area. The estimated net area must be at least 1.645 (hard-coded) times the estimated standard deviation of the baseline area for the peak to be accepted,

otherwise, it is deleted from the peak search results. If `gards_proc_params_template.area_reject` is set to “1,” peak areas must be positive to be accepted.

The peak search algorithm may find zero peaks when the ECR or RER calibrations are poor or can not be derived. A simple peak search algorithm that does not require calibration data has been added to analysis. This algorithm is only used when no peaks are found during the initial peak search. The algorithm finds spikes in the spectrum that exceed the baseline by more than three times its square root. (The baseline is the median value of 25 data points along the spectrum.) Once several peaks are found, the analysis uses these to determine the calibration of the detector [Bie00a].

The output of this function is a structure that contains, for each peak, the centroid channel, centroid channel uncertainty, centroid energy, centroid energy uncertainty, left channel, width, continuum background count, continuum background count uncertainty, FWHM, FWHM uncertainty, net area, net area uncertainty, gross area, gross area uncertainty, counts per second, counts per second uncertainty, efficiency, efficiency uncertainty, number of average background channels, and flags.

Calibration Update

Due to changes in the state of a detector, the initial ECR and RER equations may not accurately represent the current detector state. Therefore, the ECR and RER must be updated to calculate best estimates of energy and resolution values. This functionality is provided as an addition to the Canberra software. Much of the information in this section is from [Bie00a].

Changes in the ECR are commonly a result of the detector gain drifting over time. The updated ECR is automatically selected from four sources according to which is assigned the highest score. The four possible sources of ECR data include the following:

- the pair data received in the current SAMPLEPHD message,
- the MRP sample from the same detector,
- the MRP quality control count (QCPHD) from the same detector, and
- the update algorithm.

Each ECR is scored with an algorithm as defined in [Eva99a]. The ECR with the best score is chosen for peak search and nuclide identification (NID) analysis. Not all samples have a MRP QCPHD count or a MRP sample from the same detector. In these cases, an ECR is selected from the remaining sources.

ECR Update

The ECR update (ECRU) algorithm is one of four sources for updating the ECR. The update algorithm creates a new ECR by attempting to match a list of expected peaks (reflines) to those found in the sample spectrum. If enough peaks are matched, a new ECR is estimated. The input to the ECRU routine includes the following:

- the output structure from the peak area calculation;
- the detector- and station-dependent peaks expected to be observed in the spectrum, based on the PHD type (**gards_update_reflines**);
- variables from **gards_update_params_template**; and
- the peak locate results (located in the .cnf file).

When update processing begins, the reflines are retrieved from the database for the given detector (**gards_update_reflines**). For the best results, it is essential that **gards_update_reflines** contains a list of prominent lines tuned to match the characteristics of both the detector and sampling station.

The updated ECR estimate is obtained by fitting a polynomial function to a data set using QR decomposition (Q represents an orthogonal matrix; R represents an upper-right triangular matrix). The data set is a matrix that contains the matched peak centroids (in channels), their associated or ‘known’ refline energies, and estimates of the centroid uncertainties. The peak centroid uncertainties, σ_1 , are dependent upon the peak areas and are estimated using the empirical function below:

$$\sigma_1(A) = 0.01 + 8A^{-0.6}$$

where σ_1 has units of channels and A is the peak area in counts.

The update processing selects the polynomial order (up to three) using the same scoring algorithm mentioned in “[Calibration Update](#)” on page 29. There is also available the option to force a linear fitting (`gards_update_params_template.f_linear`) to the data set. Normally, the data is weighted according to the peak location uncertainties during the decomposition fitting. A weighted estimation of the ECR prevents small, poorly located peaks from having a substantial impact on the resulting fit.

After a successful ECR update, the newly estimated ECR coefficients are written to `gards_energy_cal`, overwriting the values currently stored there. If the update is unsuccessful (for example, not enough peaks/lines matched) then the original ECR coefficients stay in the `gards_energy_cal` table.

The ECRU can fail if large gain shifts cause peaks to be matched incorrectly to reflines, especially if there are unusual peaks in the spectrum. If this occurs, the peak centroid energies will be incorrect and either no nuclide identification takes place or an incorrect identification results.

The ECRU can be skipped by entering a command line override (-sk option). If this option is chosen, the RER update (RERU) is also automatically skipped. In this case, the energy and resolution coefficients, along with the energy tolerance, must be entered manually for the analysis to succeed. If updating fails, the sample spectrum is left unanalyzed (`gards_sample_status.status = 'A'`).

RER Update

Changes in the RER are commonly a result of increases in the detector crystal temperature. Crystal warming can result from a slow degradation of cooling ability or an abrupt failure in the cooling system, for example, a mechanical failure or loss of liquid nitrogen.

The RERU algorithm immediately follows the ECRU routine, and utilizes the same reline-peak matching results. An estimate of the new RER is obtained by fitting the general RER form (see “[Peak Locate](#)” on page 24) to a data set using QR decomposition. The data set is a matrix that contains matched peak widths in FWHM, associated reline energies, and estimates of the FWHM uncertainties. The FWHM uncertainties, σ_f , are determined by the following empirical equation:

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$$\sigma_f(A) = 1.9445A^{-0.4338}$$

where σ_f has the units of keV and A is again the peak area in counts. This equation was derived using peak area and FWHM uncertainties acquired by Monte-Carlo methodology.

Like the ECRU, the RERU can be skipped by entering a command line override (see “[ECR Update](#)” on page 30). The RERU can, however, be skipped without skipping the ECR update through the use of a different manual override; the `-dr` flag [IDC7.1.10Rev1].

After a successful RER update, the newly estimated RER coefficients are written to **gards_resolution_cal**, overwriting the values currently stored there. If the updating process is unsuccessful (for example, if the ECR fails), then the original RER coefficients remain in the **gards_resolution_cal** table.

Second Peak Locate, Peak Area

Inputs to this function are the same as those in the first peak locate/peak area processing, plus the updated energy and resolution coefficients. This function repeats the processing described previously for the first peak locate/peak area determination except the updated calibration coefficients are used. The result is a more accurate set of peaks and centroid energies.

The output of this function is a structure identical to that from the first peak locate/peak area determination. If the full analysis sequence completes successfully, then the data in the output structure are stored in the **gards_peaks** table.

Lookup Tolerance

The lookup tolerance calculation is used to match peaks to the potential nuclides that may have created them. The calculation is based on the average prediction error (APE) instead of the mean-squared error (MSE). The APE is a direct representation of the ECR precision and is consequently more appropriate than the MSE for the lookup tolerance calculation. Details on the calculation can be found in [Eva99].

Efficiency Conversion

In this process, the net counts per second under each peak is converted to a photon emission rate (photons per second) via the efficiency vs. energy regression (EER) equation. Here, the term “efficiency” is the fraction of emitted photons that deposit their total kinetic energy within the detector crystal, and is strongly dependent upon the photon energy as well as the detector geometry. Effects on the efficiency from the loss of photon kinetic energy within a sample (self-absorption) are assumed to be negligible.

First, the EER is constructed using the energy/efficiency pair data from the MRP CAL-IBPHD. Calibration pair data are included in all PHD messages. The model used for the EER is the “Empirical Efficiency Curve,” or

$$\ln(\epsilon) = \sum_{i=0}^n \beta_i \cdot \left[\ln\left(\frac{\beta_a}{E}\right) \right]^i$$

where ϵ is the detector efficiency in counts per photon, E is energy in keV, β_i is the coefficient set, $\beta_a = \frac{E_2 - E_1}{2}$ keV, E_1 is the smallest calibration energy in keV, and E_2 is the largest calibration energy in keV. The coefficients, β_i , are determined by fitting the model to the calibration pairs using a linear least squares method.

Due to limitations in the empirical model, the efficiency variance (and hence the efficiency uncertainty) cannot be determined. To remedy this problem, “interpolation uncertainty” values are calculated at each calibration peak energy. Used in this calculation are the measured efficiency uncertainties and the difference between the measured efficiencies and those predicted by the EER. The difficulty in estimating efficiency uncertainties affects the quality of weighted-average activity results (see [“Interference Correction” on page 40](#)).

With the peak centroid energies from the peak relocate function, the EER is used to determine the appropriate efficiency values to be used in the emission rate calculation for each peak. The resulting emission rates are not stored in the database, but are used internally in the processing.

Nuclide ID and Quantification

Activity can be calculated from emission rates by using photon intensities, or abundances. The photon intensity is the fraction of radioactive decays that result in the discharge of a photon of specific energy from a certain parent nuclide. Therefore, activities [Bq] and activity concentrations [Bq/m³] cannot be calculated from emission rates until the peaks are associated with nuclides. For accurate results, peak activities must be corrected for interferences from other isotopes.

In this section, three functions are described: nuclide identification, nuclide quantification, and interference correction. The output of these processes includes identified nuclides and corrected line activities or activity concentrations. These processes are part of the Genie-2000 Spectroscopy Tools package. Results are included in the ARR, while released versions of the results can be found in the RRR and SSREB.¹

Nuclide Identification

The NID function begins with the retrieval of data from the nuclide library (NL). The NL is a Canberra-formatted binary file (.nlb) that contains nuclide data such as half-lives, photon emissions, and abundances. The location of the NL is accessed from the .cnf file (**gards_proc_params_template.nuclide_lib**). If a nuclide is not present in the NL, it cannot be identified.

The NL used for analysis of particulate BLANKPHD, CALIBPHD, DETBKPHD, and SAMPLEPHD includes information on the following nuclides and spectral features:

- activation and fission products in the Categorization List for Particulate Samples [CTB00b];
- selected natural nuclides (primordial and cosmogenic);
- selected anthropogenic nuclides including those in common calibration sources;

1. In the [Can97] reference, the term “activity” is often used to infer “activity concentration” although these quantities are very different.

- selected nuclides to complete decay chains for progeny concentration correction; and
- recurring random-sum peaks and escape peaks.

A list of all nuclides in this NL can be found in [Bie00a].

All photon lines above 45 keV with an abundance greater than 1% of the maximum abundance for that nuclide are included in the library. To account for commonly occurring lines from certain natural radionuclides, some exceptions were made to the abundance rule. For example, anomalous thresholds were used for ^{212}Bi (0.2%), ^{212}Pb (0.3%), ^{208}Tl (0.04%), and $^{234\text{m}}\text{Pa}$ (10%). Some lines in the NL have false intensity values for facilitating the NID.

The default nuclide library used in the analysis of particulate QCPHD has been modified to have consistent format with the default nuclide library used for the other PHD types analyzed by *rms_analyze*. More information on the updated QC nuclide library can be found in [Bie01c].

The noble gas nuclide library for high-resolution gamma-ray spectroscopy detection systems was generated in the following manner. All gaseous nuclides listed in [Vla98] are included as FISSION (G) nuclides. All COSMIC nuclides in the particulate library are included as COSMIC nuclides. All NATURAL nuclides in both the particulate library and the ^{222}Rn decay chain are included as NATURAL nuclides. The methodology used in determining the nuclide properties (half-life, line energy, line abundance, and the associated uncertainties) is the same as that used in determining the particulate library nuclide properties. A list of all nuclides in this NL can be found in [Bie00b].

Suggested libraries for analysis of low-resolution and β -gated γ spectra from ARIX noble gas units are discussed in [Pop01].

To associate spectrum peaks with nuclides, the NID processing compares each nuclide in the NL to the peaks observed in the spectrum. If a peak's centroid energy matches a photon energy in the NL to within `gards_sample_proc_params.energy_tol` keV, then it is accepted. The nuclide is retained as a candidate only if it passes further testing. See Appendix A for a description of the *energy_tol* calculation.

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Test results are expressed as a confidence index (CIX) that is incrementally reduced by various penalty functions. At the beginning of the tests, the CIX of the candidate nuclide is set to one. Separate penalty functions are calculated for each of three tests and depend on the following: (1) the photon energy difference between the observed lines and those in the NL; (2) the absence of photon lines in the spectrum, taking into account abundances and efficiencies; and (3) the half-life of the candidate nuclide. See [Can97] for more details.

If, after the tests are complete, the resulting CIX (`gards_nucl_ided.comp_confid`) remains above the user defined threshold, `gards_proc_params_template.nid_confid`, then the nuclide is accepted into a matrix of possible identifications. The smaller the `nid_confid` parameter (0.1 – 1), the more numerous the acceptable nuclide candidates will be. At present, the `nid_confid` is set low to allow for the identification of many nuclides, especially natural nuclides that often have weak spectral signatures.

Nuclide Quantification

Depending on the PHD type, either activity values (BLANKPHD, CALIBPHD, DETBKPHD, or QCPHD) or activity concentrations (SAMPLEPHD) are determined. The Canberra software does not correct the progeny radionuclide activities for the decay of their parents. This offset is accounted for later in the automatic analysis sequence. See [“Parent/Daughter Calculations” on page 42](#).

The activity processing is directed by the parameter, `gards_proc_params_template.buildtype`. If the PHD type is SAMPLEPHD, then `buildtype` is automatically set to “BUILD” and the processing returns activity concentrations decay-corrected for sampling time, processing time, and acquisition time. If the PHD type is BLANKPHD, CALIBPHD, DETBKPHD, or QCPHD, then `buildtype` is automatically set to “NONE” and the processing returns activity values that are decay-corrected for decay and acquisition time.

If a nuclide is identified, all associated line activity concentrations are calculated using

$$Q = \frac{S}{V \epsilon \gamma T_1 F_B K}$$

where Q is the activity concentration in $\mu\text{Bq}/\text{m}^3$, S is the net peak area in counts, V is the air sample volume in m^3 , ε is the detector photon efficiency in counts per emitted photon, y is the photon abundance (or intensity) in photons per decay, T_1 is the live-time of the sample acquisition in seconds, F_B is a factor used to convert activity to μBq , and K is the unitless decay-correction factor. Because the sample volume appears in the denominator, the spectral analysis can fail if the sample volume is zero. K has three terms to account for decay during sampling, processing, and acquisition.

$$K = \left[\frac{1 - e^{-(\lambda t_s)}}{\lambda t_s} \right] \cdot e^{-(\lambda t_p)} \cdot \left[\frac{1 - e^{-(\lambda t_a)}}{\lambda t_a} \right]$$

where t_s is the air sampling time in seconds, t_p is the time between sampling and acquisition in seconds, t_a is the acquisition real time in seconds, and λ is the decay constant in s^{-1} ,

$$\lambda = \frac{\ln(2)}{T_{1/2}}$$

where $T_{1/2}$ is the nuclide's half-life. For particulate samples, processing consists of sample preparation and/or decay, and lasts for approximately 24 hours. The Genie-2000 software calculates decay-corrected activities by setting $V="1"$ and using the last two terms of K . All line activities and activity concentrations (*activity*) are stored in **gards_nucl_lines_ided**.

It is important to note that the efficiency, ε , used to determine activity or activity concentration values is derived from the efficiency-energy regression (EER) equation fitted to the efficiency pairs reported in the `#g_Efficiency` block of the PHD message. Therefore, it is important that the pair data reported in this block are representative of the acquisition data in the `#g_Spectrum` block. This is especially true for noble gas data from ARIX units because two spectra must be sent per sample: a low-resolution γ spectrum for identification and quantification of $^{131\text{m}}\text{Xe}$ and $^{133\text{m}}\text{Xe}$ and a β -gated γ spectrum for identification and quantification of ^{133}Xe and ^{135}Xe . In the case of the latter, the data in the `#g_Spectrum` block is the β -gated γ spectrum and the data in the `#g_Efficiency` block is the β -gated γ efficiency. See [IDC3.4.1r3] for more details.

For each nuclide in the NL, a “key” decay photon (keyline) is designated. Keylines usually have a relatively high abundance and high efficiency (lower energy) as well as minimum or zero contributions from interfering nuclides. The processing retrieves `gards_nucl_lines_ided.activity` for the key photon and writes it to `gards_nucl_ided.activ_key` as the activity of the nuclide. If an identification is made for a nuclide that is not present (this happens on occasion, particularly due to a low setting of the `gards_proc_params_template.nid_confid` parameter), the reported keyline activity can be negative.

Sometimes, relatively short-lived nuclides (for example, ^{208}Tl , $T_{1/2} = 3$ minutes) are observed in spectra because of the presence of longer-lived precursor nuclides (parent or grandparent). Daughter nuclides initially present in the sampled air may have already decayed. However, a photopeak results from the continued presence and decay of the precursor in the sample due to the presence of the parent. In a situation where the half-life of the daughter is much less than that of its parent, the daughter is observed to decay at the same rate as the parent. This is called “secular equilibrium” and is characterized by the daughter and parent nuclide having equal activities, that is,

$$\lambda_p N_p(t) = \lambda_d N_d(t)$$

where N is the number of atoms, p designates the parent nuclide, and d designates the daughter. In a system where $N_d(0) = 0$, secular equilibrium is achieved after the time, t , expressed in the following equation.

$$t = \frac{\ln(2 - \frac{\lambda_d}{\lambda_p})}{(\lambda_p - \lambda_d)}$$

Before this time has elapsed, the activity of the daughter is less than that of its parent.

In the NL, daughter nuclides in secular equilibrium with a long-lived parent are assigned artificial half-lives of 9.999 years so that they may be identified by the automated processing, which otherwise rejects the identification based on the actual decay time of the daughter nuclide. Affects of parent-daughter relationships on the activity concentration are accounted for later in the processing sequence. See [“Parent/Daughter Calculations” on page 42](#).

Other nuclides have been assigned the artificial half-life constant. These include cosmogenic radionuclides as well as those from radiation interactions with the shielding materials. Cosmogenic radionuclides are constantly being produced due to the bombardment of the earth by cosmic rays. Photons originating from the surrounding shielding materials are also produced constantly while a sample is being counted. These are due to sample radiations interacting with the shielding material atoms, producing back-scatter and X-ray peaks.

Nuclides with artificial half-lives are not quantified. Those that have been assigned the artificial half-life constant are displayed in [Table 1](#) below.

TABLE 1: NUCLIDES IN THE NUCLIDE LIBRARY ASSIGNED THE ARTIFICIAL HALF-LIFE CONSTANT

Element Symbol	Name(s) in RMS Database	Origin(s)
Ac	AC-228	natural
Ar	AR-41	activation
Ba	BA-136M	fission
Bi	BI-212, BI-214	natural
Cd	CD-113	cosmic
Cu	CU-63	cosmic
F	F-19	cosmic
Ge	GE-71M, GE-73M, GE-74, GE-75M	cosmic
Hg	HG-205	cosmic
I	I-132	fission
In	- IN-113M - IN-115M	- activation - fission
Pa	PA-234M	natural
Pb	- PB-203M, PB-204M, PB-206, PB-207M - PB-214	- cosmic - natural
Pr	PR-144	fission

TABLE 1: NUCLIDES IN THE NUCLIDE LIBRARY ASSIGNED THE ARTIFICIAL HALF-LIFE CONSTANT (CONTINUED)

Element Symbol	Name(s) in RMS Database	Origin(s)
Te	TE-129	fission
Tl	- TL-207	- cosmic
	- TL-208	- natural
Y	- Y-89M	- activation
	- Y-91M	- fission

Interference Correction

At this point in the processing, weighted average activities are determined for BLANK-PHD, CALIBPHD, DETBKPHD, and QCPHD (*buildtype* = 'NONE') while weighted average activity concentrations are determined for SAMPLEPHD (*buildtype* = "BUILD"). This function is part of the Genie-2000 Spectroscopy Tools package.

First, the peak/nuclide matrix from the NID step is checked for the presence of multiple nuclide matches to a peak. When an observed peak has contributions from more than one nuclide, the separate contributions are described as having "interference."

If interference is not detected for any of a nuclide's lines, then the nuclide's average activity or concentration (**gards_nucl_ided.ave_activ**) is calculated by a simple weighted average of the individual line activities. The line activities (or concentrations) are weighted according to their associated uncertainty. Because the activity and concentration uncertainties involve the ill-defined interpolation uncertainty from "[Efficiency Conversion](#)" on [page 33](#), the **gards_nucl_ided.activ_key** is used in place of **gards_nucl_ided.ave_activ** as the recorded activity. Considerations relating to cascade summing corrections (not yet implemented in this software release) can also affect the choice of which result to report.

If there are two or more nuclides with at least one common peak, then average weighted activities/concentrations are calculated via a weighted multiple linear regression. The solution is attempted using an unconstrained, pseudo-inverse approach in which negative elements in the estimated activity vector are not excluded during estimation. See [Can97] for details.

The output from the interference correction process includes **gards_nucl_ided.ave_activ** and **gards_nucl_ided.nid_flag** parameters for every nuclide in the NL. The *nid_flag* is “0” if a nuclide is not identified and “1” if it is. Note: when searching **gards_nucl_ided** for the nuclides found in a spectrum, either a nonzero activity or a nonzero *nid_flag* should be specified because activities are present for all nuclides (most of them are zero).

Minimum Detectable Concentration

This function is part of the Genie-2000 Spectroscopy Tools package. It determines minimum detectable activities (MDA) or MDCs for each nuclide in the NL for every spectrum depending on the PHD type. The inputs to this function include the results of the second peak search and the NID. Results are included in the ARR, while a released version of the results can be found in the RRR.

The algorithm of this function is based on a widely-accepted statistical treatment developed by Currie [Cur68]. The foundation of the method rests upon the determination of two important parameters: (1) a Critical Level, and (2) a Detection Limit. The Critical Level (L_C) is the net signal level below which an observed signal cannot be reliably detected. The Detection Level is the true net signal level which may be a priori expected to lead to detection. In general, $L_D > L_C$.

To calculate the MDA or MDC, L_C and L_D must first be determined. Without going into the derivations, these parameters are calculated using the equations below. These are valid for samples without separate background counts.

$$L_C = k \sqrt{B + (\sigma_B)^2}$$

and

$$L_D = k^2 + 2L_C$$

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where k is the confidence factor (related to the probabilities of Type I and Type II errors), B is the baseline counts, and σ_B is the uncertainty of the baseline counts. Equations for the baseline and the baseline uncertainty can be found in [“Peak Area” on page 26](#).

In the determinations of L_C and L_D , a confidence level of 95% ($k = 1.645$) is used. (The confidence level can be set in the database by changing the variable **gards_proc_params_template.nid_confid**.) Peaks with net areas less than L_C are considered not detected by the processing. This test is performed after the NID/quantification step discussed previously.

The activity concentration equation in [“Nuclide Quantification” on page 36](#) is used to calculate the MDC with L_D substituted for S . In determining MDAs, the same equation is used except V is set to 1 and only the last two terms of K are included. (Because Canberra reads MDC and MDA interchangeably, from this point forward, MDC will be used to refer to both figures.)

If an NL line has not been matched to an observed peak, then a pseudo-ROI is defined where the peak would have occurred had it been present in the spectrum. The width of this ROI is a function of the *mdc_width* parameter in **gards_proc_params_template**; the default value is 1.25 [CTB99a].

Once calculated, MDCs for all lines of the identified nuclides are written to **gards_nucl_lines_ided**. Nuclide-specific MDCs are then determined. For multi-line nuclides, the smallest MDC associated with the lines is selected as the MDC for that nuclide. These values, as well as those from single-line nuclides, are written to the **gards_nucl_ided** table for all nuclides in the NL. The binary parameter, *report_mda*, determines whether a given nuclide's MDC is to be reported in the data products. This is set so that MDCs are reported for all relevant anthropogenic nuclides.

Parent/Daughter Calculations

This function corrects the activity of nuclides that have a parent nuclide contributing to the observed counts in a sample. In some cases, all the net counts in a peak of a progeny nuclide are due to the parent's decay into the progeny. Previous versions of the automatic processing software did not correct for this effect; sometimes resulting in prepos-

terously large atmospheric activity concentrations for the progeny radionuclide. Although the longest decay chain in the NL consists of three radionuclides (see [Table 2](#)), the current software supports up to four nuclides in a decay chain.

The progeny activity correction function reads from the **gards_aux_lib**, **gards_nucl_ided**, **gards_nucl_lines_ided**, and the **gards_sample_aux** database tables. The results are written to the **gards_nucl_ided** database table, overwriting the uncorrected values. A flag is set for each line in the table that is corrected by the parent/daughter calculation process. The analyst can turn off the parent-progeny calculation with a command line parameter (-pdcalc option). The progeny activity correction function consists of two main components: the decay chain determination and the activity calculation. These are discussed in detail below.

Decay Chain Determination

The purpose of this function is to determine whether or not a decay chain is present in a sample. This is accomplished by performing the two tests described below.

1. Are all nuclides in a decay chain present in the sample? (The nuclides identified are found in **gards_nucl_ided**.)
2. Do all nuclides in the decay chain satisfy the half-life criterion? (See [Table 2](#).)

The half-life criterion is

$$\frac{t_d}{t_{1/2}} < \chi$$

where t_d is the sample decay time (the acquisition start time minus the collect stop time), $t_{1/2}$ is the radionuclide half-life found in **gards_aux_lib**, and χ is a threshold set to 12. The half-life, $t_{1/2}$, represents the actual half-life and is not necessarily the same half-life used for nuclide quantification.

TABLE 2: DECAY CHAINS IN THE NUCLIDE LIBRARY

Chain ID	Parent	Daughter	Grand-Daughter	Half-Life Criterion ¹
1	⁸⁹ Zr	^{89m} Y	-	no
2	⁹¹ Sr	^{91m} Y	⁹¹ Y	no
3	⁹⁵ Zr	⁹⁵ Nb	-	yes
4	⁹⁹ Mo	^{99m} Tc	-	yes
5	¹¹³ Sn	^{113m} In	-	no
6	¹¹⁵ Cd	^{115m} In	-	yes
7	¹²⁵ Sn	¹²⁵ Sb	-	yes
8	^{129m} Te	¹²⁹ Te	-	no
9	^{131m} Te	¹³¹ I	-	yes
10	¹³² Te	¹³² I	-	yes
11	¹³⁶ Cs	^{136m} Ba	-	no
12	¹⁴⁰ Ba	¹⁴⁰ La	-	yes
13	¹⁴⁴ Ce	¹⁴⁴ Pr	-	no
14	¹⁵⁶ Sm	¹⁵⁶ Eu	-	yes
15	^{196m} Au	¹⁹⁶ Au	-	yes
16	²¹² Pb	²¹² Bi	²⁰⁸ Tl	no
17	²¹⁴ Pb	²¹⁴ Bi	²¹⁰ Pb	no
18	²²⁸ Ac	²²⁸ Th	²²⁴ Ra	yes
19	²³⁴ Th	^{234m} Pa	-	no

1. Half-life criterion assumes a 24-hour sample decay time.

Activity Calculation

The activity is sequentially calculated for each progeny nuclide belonging to an identified decay chain. First, the parent activity is used to correct the daughter activity. Next, the parent and the corrected daughter activities are used to correct the granddaughter activity. Finally, the parent, the corrected daughter, and the corrected granddaughter activities are used to correct the great-granddaughter activity. The activity equations are derived below.

The first step in the derivation is to describe the activity of each member in the decay chain as an ordinary differential equation (ODE) as follows.

$$\frac{dA_1(t)}{dt} = Q_1F(t) - \lambda_1A_1(t)$$

$$\frac{dA_2(t)}{dt} = Q_2F(t) - \lambda_2A_2(t) + \lambda_2A_1(t)$$

$$\frac{dA_3(t)}{dt} = Q_3F(t) - \lambda_3A_3(t) + \lambda_3A_2(t)$$

$$\frac{dA_4(t)}{dt} = Q_4F(t) - \lambda_4A_4(t) + \lambda_4A_3(t)$$

where $A_1(t)$ is the time-dependent activity of the parent, $A_2(t)$ is the time-dependent activity of the daughter, $A_3(t)$ is the time-dependent activity of the granddaughter, $A_4(t)$ is the time-dependent activity of the great-granddaughter, Q_1 is the key-line atmospheric activity concentration of the parent (from **gards_nucl_ided**), Q_2 is the key-line atmospheric activity concentration of the daughter, Q_3 is the key-line atmospheric activity concentration of the granddaughter, Q_4 is the key-line atmospheric activity concentration of the great-granddaughter, $F(t)$ is the time-dependent flow rate, and λ_1 , λ_2 , λ_3 , and λ_4 are the decay constants. These equations are applied from collect start to acquisition stop. $F(t)$ is a step function that equals zero after the collect stop time.

The ODEs are numerically solved for $A_1(t)$ - $A_4(t)$ in $k-1$ iterations using the Matlab function **ode45** where k is the highest number of generations in the decay chain. The associated uncertainty is assumed to originate completely from the uncertainty in the ancestor activity, that is

$$\sigma_{A_2} = A_2 \frac{\sigma_{Q_1}}{Q_1}$$

$$\sigma_{A_3} = A_3 \sqrt{\left(\frac{\sigma_{Q_1}}{Q_1}\right)^2 + \left(\frac{\sigma_{Q_2}}{Q_2}\right)^2}$$

$$\sigma_{A_4} = A_4 \sqrt{\left(\frac{\sigma_{Q_1}}{Q_1}\right)^2 + \left(\frac{\sigma_{Q_2}}{Q_2}\right)^2 + \left(\frac{\sigma_{Q_3}}{Q_3}\right)^2}$$

During the first iteration, Q_2 , Q_3 , and Q_4 are set to zero and the ODEs are solved. The results for $A_1(t)$, $A_3(t)$ and $A_4(t)$ are neglected for the moment. The activity of the daughter during sample collection due to its parent's decay, P_2 , is determined by numerically integrating $A_2(t)$ from the collect start time to the collect stop time using the Matlab function **trapz** (trapezoidal method). This activity value is converted to atmospheric activity concentration using the equation below

$$P_2 = \frac{\lambda_2^2 A_2}{F(1 - e^{-\lambda_2 t_s})e^{-\lambda_2 t_d}(1 - e^{-\lambda_2 t_r})}$$

According to error propagation, the uncertainty of P_2 is as follows

$$\sigma_{P_2} = P_2 \sqrt{\left(\frac{\sigma_{A_2}}{A_2}\right)^2 + \left(\frac{\sigma_F}{F}\right)^2}$$

The next step determines the amount of daughter activity that can be attributed to atmospheric contents, Q_2 . Q_2 is also called the key-line activity concentration. This is calculated by subtracting the activity concentration due to parent decay, P_2 , from the total activity concentration originally determined for the key-line by the automatic analysis algorithm, T_2 , that is,

$$Q_2 = T_2 - P_2$$

This correction is also performed on each non-key-line activity concentration of the daughter. The uncertainty of Q_2 can be calculated using simple error propagation as

$$\sigma_{Q_2} = \sqrt{(\sigma_{T_2})^2 + (\sigma_{P_2})^2}$$

where σ_{T_2} is also from the automatic analysis algorithm.

Now that Q_1 and Q_2 are known, the four ODE's are solved for $A_1 - A_4$ with Q_3 and Q_4 set to zero. The activity of the granddaughter during sample collection due to its parent's decay is determined by integrating $A_3(t)$ from the collect start time to the collect stop time. P_3 is calculated and used to determine Q_3 using equations similar to those above.

Q_1 , Q_2 , and Q_3 are now known. The four ODE's are solved for $A_1 - A_4$ with Q_4 set to zero. The activity of the great-granddaughter during sample collection due to its parent's decay is determined by integrating $A_4(t)$ from the collect start time to the collect stop time. P_4 is calculated and used to determine Q_4 using equations similar to those above.

The average activity concentrations of N_1 - N_4 are calculated according to

$$\bar{Q}_i = \frac{\sum_{j=1}^J \frac{Q_i^j}{(\sigma_{Q_i^j})^2}}{\sum_{j=1}^J \frac{1}{(\sigma_{Q_i^j})^2}}$$

where the subscript 'j' represents a detected peak and 'i' is the generation number of the decay chain nuclide. The summations are over all peaks that are the key-line or that do not have interference, have an activity uncertainty greater than zero, and have an activity greater than the activity uncertainty. The key-line activity, the average activity, and the associated uncertainties are saved to **gards_nucl_ided**.

▼ Automatic Processing

ANALYSIS OF 3-D BETA-GAMMA COINCIDENCE DATA

This section describes the analysis algorithm applied to radionuclide PHD from sites employing 3-D β - γ coincidence detection. The processing code analyzes this data type only. The analysis program is called *rms_xanalyze* and a simplified diagram of the processing steps is illustrated in [Figure 8](#) below. For a more detailed schematic, see Chapter 7 in [IDC7.1.10].

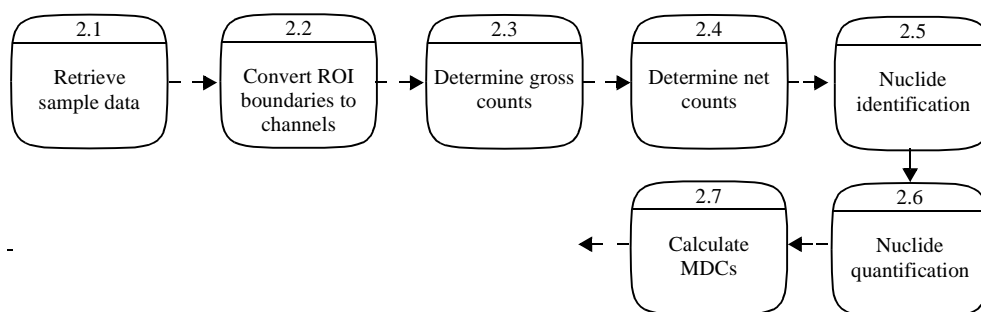


FIGURE 8. AUTOMATIC PROCESSING OF 3-D β - γ COINCIDENCE DATA

Rms_xanalyze begins by reading the processing parameters and the 3-D spectral data from the database. The histogram is divided into ROIs defined by the γ -ray energies and β -energies reported in the PHD message. The gross counts in each ROI are calculated by summing the counts per channel. The net counts are calculated by correcting the gross counts for the affects of Compton continuum background, detector background, gas cell background (the "memory effect"), and interference from other nuclides. Four of these nuclides ($^{131\text{m}}\text{Xe}$, ^{133}Xe , $^{133\text{m}}\text{Xe}$, and ^{135}Xe) are used to categorize the spectrum. The calculated air concentration and MDC for each categorization nuclide are determined using the net counts and the processing parameters. Each of these processing steps are described in detail below.

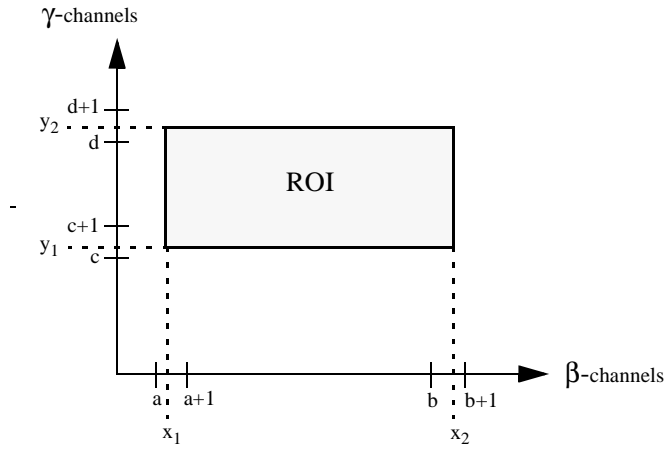
Convert ROI Boundaries to Channels

The software begins by extracting 3-D β - γ coincidence data and the associated processing and sample parameters from the database. The spectral data are stored in channels whereas the ROI boundary definitions are stored in energy units. The ROI boundaries from the `#ROI_Limits` block of the PHD message are converted to channels using the inverse ECR like that described in “Peak Locate” on page 24. An ECR is determined by fitting the calibration pair data reported in the PHD file using QR Decomposition. The pair data are those reported in the `#g_Energy` and `#b_Energy` blocks. The form of the ECR (linear or quadratic) can be chosen on a per station basis via the `beta_ecr_order` and `gamma_ecr_order` fields in the `gards_sample_xe_procs_params` and `gards_xe_procs_params_template` tables. It is recommended to use a quadratic equation for the β ECR for data from SAUNA units. Linear equations are recommended for all other ECR types.

Determine Gross Counts

After the ROI boundaries are converted from energy to channel units, the gross counts in each ROI (G) are determined by summing the counts ($C_{i,j}$) in each channel within the ROI boundaries. Because the calculated boundary channels are real numbers and not integers, a ROI boundary typically falls within the middle of a channel as illustrated in [Figure 9](#). Hence, the counts within the boundary channels are weighted by the percentage of the boundary channel that is located within the ROI. An equation describing this calculation is below.

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**FIGURE 9. ROI CHANNEL BOUNDARIES**

$$G = \sum_{i=a}^b \sum_{j=c}^d f_{\beta} \cdot f_{\gamma} \cdot C_{i,j}$$

where

$$f_{\beta} = \begin{cases} a+1-x_1 & \text{for } i=a \\ x_2-b & \text{for } i=b \\ 1 & \text{for } i \neq a \neq b \end{cases}$$

and

$$f_{\alpha} = \begin{cases} c+1-y_1 & \text{for } j=c \\ y_2-d & \text{for } j=d \\ 1 & \text{for } j \neq c \neq d \end{cases}$$

Determine Net Counts

The net counts (N) are calculated by correcting the gross counts (G) for the affects of Compton continuum background (B), gas cell background, (M), detector background (D), and interference from other nuclides (I).

$$N = G - B - M - D - I$$

Compton Continuum Background

The Compton continuum counts, B, are background counts that exist in the ROI due to Compton photons counted in coincidence with electrons. The Compton background is only a concern along the γ -axis and not along the β -axis. Two Compton regions are defined per ROI: one at higher γ -channels (the upper region) and one at lower γ -channels (the lower region). [Figure 10](#) shows an example of the upper and lower Compton regions. The boundaries of the upper Compton region are the ROI β -boundaries, x_1 and x_2 ; the upper ROI γ -boundary, y_2 ; and the upper ROI γ -boundary plus n channels, y_2+n . Likewise, the boundaries of the lower Compton region are the ROI β -boundaries, x_1 and x_2 ; the lower ROI γ -boundary, y_1 ; and the lower ROI γ -boundary minus n channels, y_1-n . The variable, n, is a user-definable integer that can be set from zero to five; however, the default value for n is three. The corresponding database field for n is *compton* in **gards_sample_xe_procs_params** and **gards_xe_procs_params_template** tables. To define n for a station, *compton* needs to be set in **gards_xe_procs_params_template**.

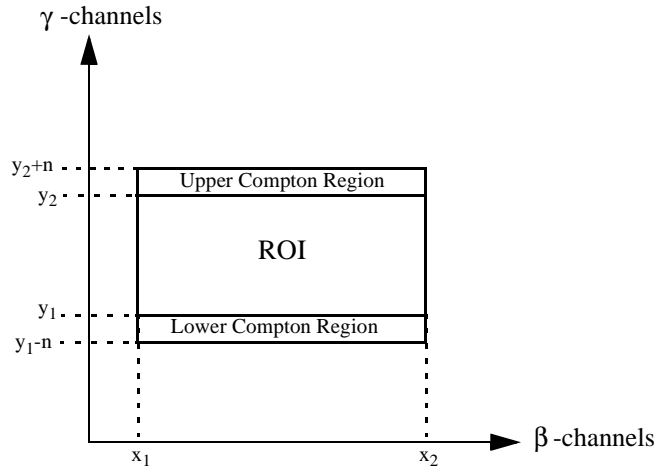


FIGURE 10. UPPER AND LOWER 2-D COMPTON REGIONS (NOT TO SCALE)

Using the Compton region boundaries, the counts in each region are calculated in the same manner as the gross counts. (See [“Determine Gross Counts”](#) on page 49.) The Compton counts in the ROI are then determined by summing the counts from the upper and lower Compton regions (B_1 and B_2 , respectively) and multiplying this sum by the ratio of the ROI area to total Compton area as demonstrated in the equation below.

$$B = \frac{(x_2 - x_1) \cdot (y_2 - y_1)}{((x_2 - x_1) \cdot (y_1 - (y_1 - n))) + ((x_2 - x_1) \cdot ((y_2 + n) - y_2))} \cdot (B_1 + B_2)$$

This equation simplifies to

$$B = \frac{(y_2 - y_1)}{2n} \cdot (B_1 + B_2)$$

Gas Cell Background

The gas cell background, M , comprises extra counts resulting from the adsorption of some of the previous sample gas onto the gas cell walls. It is often called the memory effect. As shown by the equation below, the gas background counts are calculated by

multiplying the net ROI counts of the MRP gas background sample, N_{GB} , by several decay factors. The decay factors account for differences in acquisition time between the two samples and for the decay of the radionuclide between acquisitions. A gas background sample is measured prior to every sample measurement.

$$M = \frac{N_{GB}}{(1 - e^{-\lambda t_{GB}})} \cdot e^{-\lambda t_{GB}} \cdot (1 - e^{-\lambda t_r})$$

In this equation, t_{GB} is the real acquisition time of the gas cell background count, and t_r is the real time of the current sample's detector acquisition time.

Detector Background

The detector background, D , comprises extra counts deposited by radiation originating from anthropogenic radionuclides located outside the detector or cosmogenic radionuclides. The detector background counts are calculated by multiplying the net counts of the MRP detector background sample, N_D , by the ratio of the live time of the current sample, t_l , to the live time of the MRP detector background sample, t_D .

$$D = \frac{t_l}{t_D} \cdot N_D$$

A detector background sample is measured only occasionally with relatively long acquisition times and with a new gas cell or one that has not been used in an amount of time for the memory effect to be significant.

Interference

A decaying radionuclide may produce counts in multiple ROIs due to possible multiple photon lines. A ROI, by definition, is only associated with the radionuclide it is used to quantify. The current ROI to radionuclide association is shown in [Table 3](#) and is illustrated in [Figure 11](#).

TABLE 3: ROIs in β - γ Coincidence Spectra Relevant to CTBT Monitoring

ROI Number	Nuclides Possible	Quantification Nuclide	Centroid γ -Energy (keV)	Centroid β -Energy (keV)
1	^{214}Pb	n/a ¹	352	-
2	^{135}Xe , ^{214}Pb	^{135}Xe	250	-
3	^{133}Xe , ^{214}Pb	^{133}Xe	81	-
4	$^{131\text{m}}\text{Xe}$, ^{133}Xe , $^{133\text{m}}\text{Xe}$, ^{214}Pb	none ²	30	-
5	$^{131\text{m}}\text{Xe}$, ^{133}Xe	$^{131\text{m}}\text{Xe}$	30	130
6	$^{133\text{m}}\text{Xe}$, ^{133}Xe	$^{133\text{m}}\text{Xe}$	30	199

1. The counts in this ROI are used only for determining interference from ^{214}Pb in ROIs #2 and #3.
2. This ROI will likely be used in the future with ROI #3 for quantification of ^{133}Xe .

Interference counts, I , are calculated by multiplying the net counts in the interfering radionuclide's associated ROI, N_I , by an interference ratio, R , as shown below.

$$I = R \cdot N_I$$

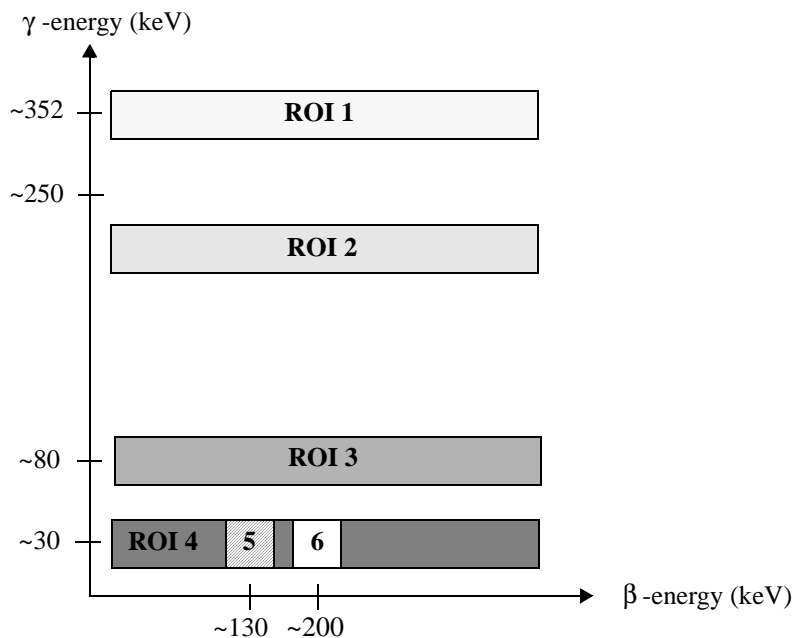


FIGURE 11. RELEVANT ROIs IN β - γ COINCIDENCE DATA ANALYSIS

The interference ratios are reported in the `#Ratios` block of a PHD file. R is equal to the ratio of the counts in the current ROI to counts in the associated ROI of the interfering radionuclide. The interference ratio is a calibration parameter that is determined experimentally before the current measurement and depends on the ROI boundaries. See [IDC3.4.1Rev2] for more information on interference count ratios.

Nuclide Identification

In *rms_xanalyze*, radionuclides are considered present if the net counts are greater than the critical limit, L_c . The derivation of L_c for 3-D β - γ coincidence systems is based on the Currie methodology [Cur68] and is detailed in [Bie01b].

Nuclide Quantification

Nuclide quantities are reported only for categorization nuclides (that is, ^{131m}Xe , ^{133}Xe , ^{133m}Xe , and ^{135}Xe) that have net counts above the critical limit. The equation used to determine the air concentration of radioxenons, Q [mBq/m³], is very similar to that for high resolution γ -spectroscopy data. It is below.

$$Q = \frac{N\psi t_s t_r}{\epsilon_{\beta\gamma} I_{\beta\gamma} V_{\text{Xe}} \xi Z t_l}$$

Here, N is the net counts in an ROI, ψ is the concentration of elemental Xe in the atmosphere, i.e., 0.087 cm³/m³; t_s is the sample collection time in seconds (s); t_r is the real acquisition time in seconds; t_l is the acquisition live time in seconds; $\epsilon_{\beta\gamma}$ is the beta-gamma coincidence detection efficiency for the electron-photon pair; $I_{\beta\gamma}$ is the abundance (or intensity) of the electron-photon pair; V_{Xe} is the sample volume of Xe in cm³; ξ is the factor required to convert activity to mBq (1Bq/1000mBq); and Z is a collection of decay factors given by the equation below.

$$Z = \left(\frac{1 - e^{-\lambda t_s}}{\lambda} \right) \cdot e^{-\lambda t_p} \cdot \left(\frac{1 - e^{-\lambda t_r}}{\lambda} \right)$$

In this equation, t_p is the decay time during processing (the time between sample collection and sample acquisition) in seconds, and λ is the decay constant in s⁻¹.

The uncertainty of Q (σ_Q) is determined by simple error propagation methodology according to the equation below.

$$\sigma_Q = Q \sqrt{\left(\frac{\sigma_N}{N} \right)^2 + \left(\frac{\sigma_\psi}{\psi} \right)^2 + \left(\frac{\sigma_{\epsilon_{\beta\gamma}}}{\epsilon_{\beta\gamma}} \right)^2 + \left(\frac{\sigma_{I_{\beta\gamma}}}{I_{\beta\gamma}} \right)^2 + \left(\frac{\sigma_{V_{\text{Xe}}}}{V_{\text{Xe}}} \right)^2}$$

In the case where both ^{133m}Xe and ^{133}Xe are identified, the calculated concentration of ^{133}Xe (Q_{133}) is corrected by the following equation to account for the parent-daughter relationship between these two nuclides.

$$Q = (G_1 + G_2)$$

In this equation, Q is the corrected concentration of ^{133}Xe and G_1 and G_2 are defined in the equations below [Bie01a].

$$G_1 = \frac{Q_{133m}\lambda_{133}}{(1 - e^{-\lambda_{133}t_s})} \left[\frac{\lambda_{133m}(1 - e^{-\lambda_{133}t_s}) - \lambda_{133}(1 - e^{-\lambda_{133m}t_s})}{\lambda_{133m}(\lambda_{133m} - \lambda_{133})} \right]$$

$$G_2 = \frac{Q_{133m}(\lambda_{133})^3}{\lambda_{133m}(\lambda_{133} - \lambda_{133m})} \frac{(1 - e^{-\lambda_{133m}t_s})}{(1 - e^{-\lambda_{133}t_s})e^{-\lambda_{133}t_p}(1 - e^{-\lambda_{133}t_r})}$$

$$\left[\frac{e^{-\lambda_{133m}t_p}}{\lambda_{133m}}(1 - e^{-\lambda_{133m}t_r}) - \frac{e^{-\lambda_{133}t_p}}{\lambda_{133}}(1 - e^{-\lambda_{133}t_r}) \right]$$

Here, Q_{133m} is the activity concentration of ^{133m}Xe in mBq/m^3 , λ_{133} is the decay constant for ^{133}Xe , and λ_{133m} is the decay constant for ^{133m}Xe .

The uncertainty of Q_{133} when ^{133m}Xe is present is determined by error propagation methodology according to the following equation.

$$\sigma_{Q_{133}} = \left[\left(\frac{Q_{133}\sigma_{N_{133}}}{N_{133}} \right)^2 + \left(\frac{Q_{133}\sigma_{\psi}}{\psi} \right)^2 + \left(\frac{Q_{133}\sigma_{\epsilon_{\beta\gamma}}}{\epsilon_{\beta\gamma}} \right)^2 + \left(\frac{Q_{133}\sigma_{I_{\beta\gamma}}}{I_{\beta\gamma}} \right)^2 + \left(\frac{Q_{133}\sigma_{V_{\text{Xe}}}}{V_{\text{Xe}}} \right)^2 \right. \\ \left. + \left(\frac{\sigma_{Q_{133m}}}{Q_{133m}} \right)^2 (G_1 + G_2)^2 \right]^{\frac{1}{2}}$$

Calculate MDCs

Rms_xanalyze determines the MDCs for radioxenons according to the following equation.

$$\text{MDC} = \frac{L_D}{\frac{\epsilon_{\beta\gamma} I_{\beta\gamma} V}{\lambda^2} (1 - e^{-\lambda t_s}) e^{-\lambda t_p} (1 - e^{-\lambda t_r})}$$

where L_D is the detection limit and F is the collection flow rate in standard cubic meters (SCM) per second. The L_D is calculated using the same equation listed in “Minimum Detectable Concentration” on page 41, that is,

$$L_D = k^2 + 2L_C$$

However, for noble gas samples acquired via β - γ coincidence, L_C is determined with a different equation because there are more sources contributing signals. The general equation used for L_C is as follows.

$$L_C = k \sqrt{B + M + I + (\sigma_B)^2 + (\sigma_M)^2 + (\sigma_I)^2}$$

Expressions for the nuclide-specific B , M , I , $(\sigma_B)^2$, $(\sigma_M)^2$, and $(\sigma_I)^2$ can be found in [Bie01b].

QUALITY CONTROL TESTS

This function has been provided as an addition to the Canberra software and is designed to run on QCPHD containing high-resolution γ -spectrometry data from a particulate radionuclide station or site. The inputs to this function are the output from the second peak search and NID steps.

Four tests are performed including two peak location tests, one resolution (width) test, and one area (efficiency) test. The purpose of the tests is to detect changes in the operating characteristics of the detector. The results of these tests are written to the **gards_qchistory** table. Notification messages are sent to subscribers when the tests fail or when test statistics fall outside of expected ranges.

Location Tests

The following tests are designed to detect large, abrupt shifts in peak locations.

Normalized Gain Test

First the code identifies the two peaks in the QCPHD that are separated by the largest distance. The centroid location of the peaks, both in channel (C_i) and in keV (E_i), are used to calculate the gain, g , via the equation below [Eva97].

$$g = \frac{C_2 - C_1}{E_2 - E_1}$$

The gain is normalized to a perfectly linear detector; that is,

$$G = g \cdot \frac{\Delta_C}{\Delta_E}$$

where Δ_C is the total number of channels in the spectrum and Δ_E is the energy span in keV.

The absolute value of the difference in the normalized gains between the last QCPHD on the detector and the present one is compared to a fixed value (`gards_qcparams.gain-change` = 0.0001) determined by analysis of historical data.

⁴⁰K Location Test

The code locates the centroid for the naturally-occurring ⁴⁰K peak, and determines its uncertainty using the empirical equation described previously in “[ECR Update](#)” on [page 30](#). The absolute value of the difference in the ⁴⁰K peak centroid location between the last QCPHD on the detector and the present one is compared to a multiple (`gards_qcparams.sdmult` = 3) of its standard deviation.

Resolution Test

The purpose of this test is to detect large changes in the detector resolution. For a more detailed discussion on this test, see [Eva97].

The FWHM and its variance are determined for all peaks in the QCPHD spectrum. These results, along with target values for these parameters (`gards_targets`), are used to produce a Chi-squared test statistic, X , as follows:

$$X = \sum_{i=1}^P \frac{(x_i - \mu_i)^2}{\xi \sigma_i^2}$$

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where p is the number of peaks, x is the FWHM of peak i in channels, μ_i is the target value for the FWHM at peak i , σ_i^2 is the variance in the FWHM of peak i , and ξ is the standard deviation inflation factor, **gards_qcparams.width_adj**. The variance of the FWHM is determined using the square of the equation in “RER Update” on page 31. ξ is a user-defined constant and permits control over the false-alarm rate. It usually ranges from 0.75 to 1.5.

The value returned for X is compared to the positive and negative 99% confidence bounds that surrounds the known mean value, $\bar{X} = p$. If X falls outside of the confidence bounds, then the test returns a FAIL result.

Area Test

The purpose of this test is to detect large changes in the detector efficiency. For a more detailed discussion on this test, see [Eva97].

The area and its variance are determined for all peaks in the QCPHD spectrum. These results, along with target values for these parameters (**gards_targets**), are used to produce a Chi-squared test statistic, X , as follows:

$$X = \sum_{i=1}^p \frac{(x_i - \mu_i)^2}{\xi \sigma_i^2}$$

where p is the number of peaks, x is the area of peak i in counts, μ_i is the target value for the area of peak i , σ_i^2 is the variance in the area of peak i , and ξ is the standard deviation inflation factor, **gards_qcparams.area_adj**. The variance of the area is calculated by the equation below.

$$\sigma_i^2 = A_i e^{\lambda_i t}$$

where A_i is the target area for peak i and λ_i is the decay constant of the peak nuclide. ξ is a user-defined constant and permits control over the false-alarm rate. It is currently set to 1.5.

The value returned for X is compared to the positive and negative 99% confidence bounds that surrounds the known mean value, $\bar{X} = p$. If X falls outside of the confidence bounds, the test returns a FAIL result.

PRIORITIZATION

This function has been provided as an addition to the Canberra software. Both particulate and noble gas FULL SAMPLEPHD are assigned priority levels. The software automatically prioritizes a sample based on the amounts and types of radionuclides identified. The results of the prioritization step are stored in the database and alert messages are sent to subscribers based on the results.

Statistical Filters

There is now the ability to choose one of two statistical filter methods on a per nuclide, per station basis: the “Exponentially-Weighted Moving Average” (EWMA) method or the Recent Distribution Comparison (RDC) method. The method is indicated in the *method_type* field in **gards_cat_template**. Both methods determine a range of concentrations for each nuclide. If the sample nuclide concentration falls within the range, it is considered normal. If the sample nuclide concentration falls outside of this range, it is considered anomalous. The statistical filters are automatically updated when an analyst releases a sample using Inspectra or CORIANT [IDC6.2.6Rev1]. Each statistical filter methodology is described below.

Exponentially Weighted Moving Average

The EWMA method relies on a time series forecasting filter to determine if an observed airborne concentration of a nuclide is consistent with previous measurements of that nuclide at that sampling station. In forecasting and applied statistics, this method is called an “Exponentially-Weighted Moving Average” (EWMA). In other engineering contexts it could be considered a very simple case of a fixed-gain Kalman filter.

The decision process is governed by equations that define a prediction interval filter (PIF). For a more details on the PIF equations, see [Eva96]. The operation of the PIF is separated into two phases: initialization and update. Six concentration data points are required to initialize the recursive filters. Once the PIF has been initialized, there should be no need to do it again except in the case of an extended break in the collection of data. Nuclide concentrations are compared to the filter states whenever new data are received.

Recent Distribution Comparison

The RDC algorithm first determines if a nuclide has been detected at a station at least three times in the past 30 days. If not, then a detected nuclide is automatically considered anomalous. If so, then the algorithm takes the last 10 activity concentrations of a nuclide at a particular station, determines the mean, and then uses a predefined abscissa value which counts how many standard deviations of the mean within which the current activity may fall without being anomalous. If the current activity concentration falls out of this range, then the nuclide detection is considered anomalous. Also, if there are not 10 previous activities the nuclide is considered anomalous.

Unlike the EWMA method, the RDC algorithm is not dependent on the sequence with which samples are received. This is a benefit; however, the RDC and EWMA algorithms regularly arrive at different categorization results for the same nuclides. If the categorization methods are not implemented in a consistent manner, this disparity can cause confusion and perhaps inaccurate categorization of samples .

Nuclide Prioritization

The first step in the sample prioritization process is to assign a priority level to each nuclide found present in a sample. This is done by determining whether each nuclide

1. has a statistical filter established for the appropriate sampling station (stored in the **gards_nic_init** table), and
2. is a relevant anthropogenic radionuclide as listed in **gards_relevant_nuclides**.

Nuclides are assigned priority levels according to the following scheme:

- Level 1

- A non-relevant anthropogenic or natural nuclide with an activity concentration that falls within its statistical filter range
- A natural nuclide that does not have a pre-established statistical filter
- Level 2 (not applicable to noble gas samples)
 - A non-relevant anthropogenic or natural nuclide with an activity concentration that falls outside of its statistical filter range
 - A non-relevant anthropogenic radionuclide that does not have a pre-established statistical filter
- Level 3

A relevant anthropogenic nuclide that falls within its statistical filter range
- Level 4
 - A relevant anthropogenic radionuclide that falls outside of its statistical filter limits
 - A relevant anthropogenic radionuclide that does not have a pre-established statistical filter

If an anthropogenic radionuclide has no pre-established statistical filter, it is considered to be present at an atypical level. It is not possible to assign a priority level of 2 to a nuclide in a noble gas sample because natural nuclides cannot be quantified. This is because noble gas stations actively separate all non-xenon elements from the air. The collection efficiency for non-xenon elements is not reported; hence, the counts detected from natural radionuclides cannot be converted to air activity concentrations. Nuclides in noble gas samples can only be prioritized as level 1, 3, or 4.

Nuclide priority levels are stored in `gards_nic.category`. The relevant anthropogenic nuclides are displayed in [Table 4](#) below. All are fission products except ^{134}Cs , which is an activation product.

TABLE 4: RELEVANT ANTHROPOGENIC NUCLIDES

Element Symbol	Name(s) in Database
Ag	AG-106M, AG-108M, AG-110M, AG-111
As	AS-74, AS-76
Au	AU-196, AU-196M, AU-198
Ba	BA-133, BA-140
Cd	CD-115, CD-115M
Ce	CE-141, CE-143, CE-144
Co	CO-57, CO-58, CO-60
Cr	CR-51
Cs	CS-132, CS-134, CS-136, CS-137
Eu	EU-152, EU-152M, EU-155, EU-156, EU-157
Fe	FE-59
Ga	GA-72
I	I-130, I-131, I-133, I-135
Ir	IR-190, IR-192
K	K-42
La	LA-140
Mn	MN-54
Mo	MO-99
Na	NA-24
Nb	NB-95
Nd	ND-147
Np	NP-239
Pb	PB-203
Pd	PD-112

TABLE 4: RELEVANT ANTHROPOGENIC NUCLIDES (CONTINUED)

Element Symbol	Name(s) in Database
Pm	PM-149, PM-151
Pr	PR-145
Rb	RB-84, RB-86
Rh	RH-102, RH-105
Ru	RU-103, RU-106
Sb	SB-120, SB-122, SB-124, SB-125, SB-126, SB-127, SB-128
Sc	SC-46, SC-47
Sm	SM-153, SM-156
Sn	SN-125
Sr	SR-91
Tc	TC-99M
Te	TE-129M, TE-131M, TE-132
Tm	TM-168
U	U-237
W	W-187
Xe	XE-131M, XE-131, XE-133, XE-133M, XE-135
Y	Y-88, Y-91, Y-93
Zn	ZN-65, ZN-69M
Zr	ZR-89, ZR-95, ZR-97

Sample Prioritization

Once priority levels have been assigned to all quantified nuclides, the sample itself is prioritized. Samples are prioritized as follows:

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- Level 1
The sample contains only Level 1 nuclides.
- Level 2 (not applicable to noble gas samples)
The sample contains one or more Level 2 nuclides. Any number of Level 1 nuclides may also be present.
- Level 3
The sample contains one or more Level 3 nuclides. Any number of Level 1 and/or Level 2 nuclides may also be present.
- Level 4
The sample contains one or more Level 4 nuclides of which only one can be a fission product. Any number of Level 3, Level 2, and/or Level 1 nuclides may also be present.
- Level 5
The sample contains two or more Level 4 nuclides, at least two of which are fission products.

Because it is not possible to have level 2 nuclides in a noble gas sample, it is impossible to have a noble gas sample assigned a priority level of 2. Noble gas samples can only be assigned priority levels of 1, 3, 4, and 5.

Once a sample has been categorized, the sample priority level is stored in **gards_sample_status.auto_category**, and the **gards_nic.sample_status** is assigned the letter "C." If a sample has been categorized as a Level 2, 4, or 5, subscribers are automatically sent a notification message. (Notification subscriber information is retrieved from the **gards_notify** table in the database.)

DATABASE FLAGS

This function has been provided as an addition to the Canberra software and runs only on FULL SAMPLEPHD containing particulate sample data. This process consists of various Data Quality and Event Screening tests that are performed on the sample. Test results are written to the **gards_sample_flags** table and are included in the ARR. Released results can be found in the RRR and SSREB data products.

These tests were created to monitor the following:

- the state-of-health of station instruments,
- the reliability of incoming data, and
- the number and frequency of certain anthropogenic nuclides observed at each station.

Data Quality Tests

The Data Quality tests compare flow rate, ^{140}Ba MDC, ^7Be FWHM, ^{40}K Location Difference, and Normalized Gain Difference values to threshold values from the **gards_flags** table. To perform the Data Quality tests, answers to the following questions are determined.

1. Is the flow rate greater than $500 \text{ m}^3/\text{hr}$?
2. Is the ^{140}Ba MDC less than $30 \mu \text{ Bq/m}^3$?
3. Is the ^7Be FWHM less than 1.7 keV ?
4. Is the ^{40}K Location Difference less than a multiple (**gards_qcparams.sdmult**) of the ^{40}K Location Difference standard deviation?
5. Is the Normalized Gain Difference less than the arbitrary constant, **gards_qcparams.gainchange**?

The first three tests are indicative of various aspects of station and detector performance. The values calculated and stored in the database for the flow rate, ^{140}Ba MDC, and ^7Be FWHM are compared to the test conditions.

The fourth test is very similar to that described previously in [“ \$^{40}\text{K}\$ Location Test” on page 59](#). The difference between the centroid location for the ^{40}K peak in the current spectrum and the location of the ^{40}K peak in the MRP spectrum is determined. The empirical formula in [“ECR Update” on page 30](#) is used to estimate the 1σ uncertainty in the ^{40}K location. The upper bound for this test is a multiple (currently 3) of this estimated standard deviation. The test is designed to detect a possible zero-shift in the detector.

▼ Automatic Processing

The fifth test is very similar to that described previously in “Normalized Gain Test” on page 58. The difference between the normalized gain for the current spectrum and that of the MRP spectrum is determined. The absolute value of this difference is compared to an arbitrary constant limit (currently set to 0.0001). The test is designed to detect a possible gain shift in the detector.

Event Screening Tests

The Event Screening tests examine whether activation products, fission products, and ^{137}Cs are observed in a sample spectrum. The event screening tests are as follows:

- 1a. Are there relevant activation products in the spectrum?
- 1b. If yes, what is the time interval since the last observation of relevant activation products at this station?
- 2a. Is there one relevant fission product present in the spectrum?
- 2b. If yes, what is the time interval since the last observation of at least one relevant fission product at this station?
- 3a. Are there two or more relevant fission products in the spectrum?
- 3b. If yes, what is the time interval since the last observation of two or more relevant fission products at this station?
- 4a. Is ^{137}Cs present in the spectrum?
- 4b. If yes, how often has ^{137}Cs been observed in the last 30 days?

Tests 1a, 2a, 3a, and 4a are the primary event screening tests. If the primary tests are TRUE, tests 1b, 2b, 3b, and 4b will be evaluated. The results of the primary tests will always appear on the RRR, ARR, and SSREB reports for particulate samples. The output of the secondary tests will only appear if the primary tests are true.

CREATING AUTOMATED RADIONUCLIDE REPORTS

The ARR Report function has been provided as an addition to the Canberra software and is processed only for FULL SAMPLEPHD data types. Inputs to this function include various data from the database.

After the Database Flags function is complete, the ARR Report function is initiated. The purpose of this CSC is to create Automated Radionuclide Reports (ARRs) for each sample that has been categorized and for which **gards_detectors.status** = "Y," indicating a primary detector was used. ARR Report collects sample information from the database for a given sample ID, and arranges the data in a text file. See [IDC3.4.1Rev2] for a complete description of the contents of the ARR, as well as for examples from both particulate and noble gas stations. The ARR is available by request and subscription via the AutoDRM [IDC3.4.1Rev2], and through the PIDC home page on the Web [IDC7.1.10Rev1].

Data Timeliness and Availability Flags

As part of the particulate ARR function, five data timeliness and availability tests are performed. The inputs to this function are data obtained from the database. The test results are displayed in the ARR and RRR for particulate samples; however, they are not written to the database. The purpose of the tests is to verify that a sample has been collected, decayed, acquired, and transmitted within the required time limits specified in the IMS Operations Manual [CTB00c]. The tests are described below. If the tests pass, then the word "YES" is displayed after the question posed above. Otherwise, the word "NO" is displayed.

1. Previous sample present?

This test determines if there is a previous sample from this station and detector without time constraints.

2. Collection time within 24 hours +/- 10%?

This test determines if the difference between *collect_stop* and *collect_start* in **gards_sample_data** is equal to or between 21.6 hours and 26.4 hours.

3. Acquisition time >= 20 hours?

This test determines if the difference between *acquisition_stop* and *acquisition_start* in **gards_sample_data** is greater than or equal to 20 hours.

4. Decay time <= 24 hours?

This test determines if the difference between *acquisition_start* and *collect_stop* in **gards_sample_data** is less than or equal to 24 hours.

5. Sample received within 72 hours of collect start?

This test determines if *entry_date* in **gards_sample_status** is less than 72 hours after *collect_start* in **gards_sample_data**.

Chapter 3: Interactive Analysis

This chapter describes the scientific premises behind the design of the interactive analysis tools and includes the following sections:

- [Overview](#)
- [MAR Tool](#)
- [Inspectra](#)
- [CORIAN](#)
- [Trendvue](#)
- [Analyst Work Area](#)
- [RMS Workflow](#)
- [Data Workbench](#)
- [Processing Tools](#)

Chapter 3: Interactive Analysis

OVERVIEW

A set of software tools are used for the interactive analysis process. This set includes the Multiple Analyst Review (MAR) Tool, Inspectra, CORIANT, Trendvue, Analyst Work Area, Radionuclide Workflow, Data Workbench, and Processing Tools. This chapter includes discussions on the scientific concepts that are integrated into these software packages. Additional information on the interactive analysis tools can be found in [IDC6.2.6Rev1], [IDC6.5.10Rev1], and [IDC7.1.10Rev1].

MAR TOOL

The purposes of the MAR Tool are to automatically manage resource allocation for sample analysis and to assign permissions to roles. This functionality enables the assignment of roles to personnel, the automatic queuing of samples for analysts, and the subsequent passing of difficult samples to other personnel in the chain of command. The tool is not equipped to perform any data analysis.

INSPECTRA

Depending on the roles assigned to a user, this software tool allows one to view sample spectra acquired from detectors employing high resolution gamma spectrometry, view other sample data, reanalyze sample spectra, categorize a sample, and add comments to a sample. This section discusses the scientific premises used in the Inspectra software tool.

Plotting a Spectrum Baseline

The baseline equations in Figure 8 on page 43 are used during automatic analysis in determining net peak areas. When plotted, the baseline would appear as discrete steps instead of as a continuous function. To display a more realistic representation of the baseline, the equivalent continuous function below is used by Inspectra when plotting peaks.

$$\text{baseline}(x, L, R) = (1 - \alpha(x))L + \alpha(x)R$$

where x represents the channel axis, L is the average counts of the three channels immediately adjacent to the left of the ROI, R is the average counts of the three channels immediately adjacent to the right of the ROI, and α is a weighting function calculated as shown below:

$$\alpha(x) = \frac{\sum_{i=1}^n \sigma_i \cdot h_i \cdot \left[1 - \text{erf}\left(\frac{1}{\sqrt{2}} \cdot \frac{x - \mu_i}{\sigma_i}\right) \right]}{2 \cdot \sum_{i=1}^n (h_i \cdot \sigma_i)}$$

where n is the total number of peaks in the ROI, h_i is the height of peak i in counts, σ_i is the standard deviation of peak i in channels, and μ_i is the centroid location of peak i in channels. A derivation of this equation is provided in Appendix A.

Calibration Plots

The calibration plots available include an energy discrepancy plot (Energy Function Plot) as well as plots for the detector resolution and efficiency (Resolution Function Plot and Efficiency Function Plot, respectively).

Energy Function Plot

The energy vs. channel equation is estimated as described in “Calibration Update” on page 24. The equation is a polynomial function that has been fitted to the reline peak centroids (in channels), their associated energies, and centroid uncertainties. Relines are both station and detector dependent and can be found in **gards_update_relines**.

A graphical representation of the ECR plot is not made available since it appears as a straight line and is therefore uninformative. Instead, a discrepancy plot is included (see [Figure 12](#)).

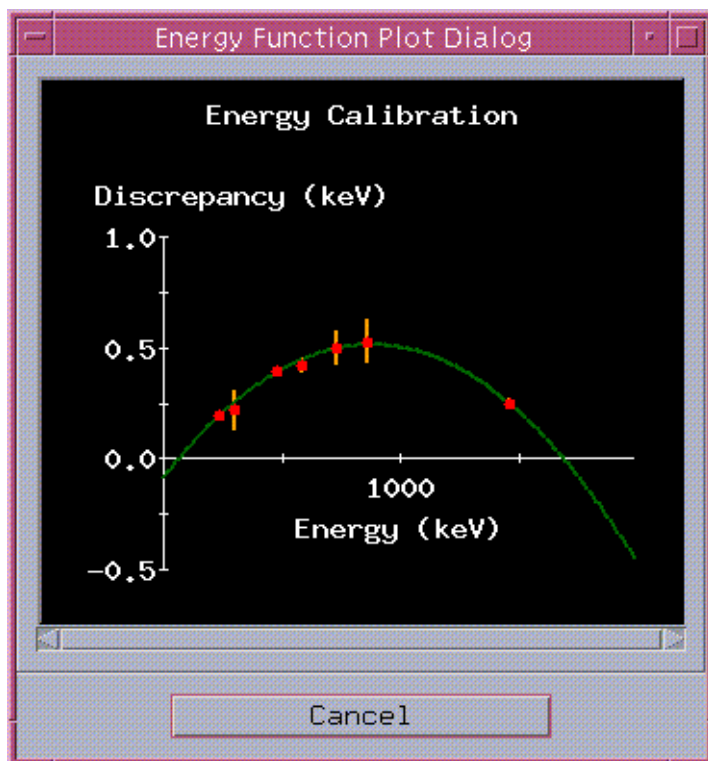


FIGURE 12.INSPECTRA DISCREPANCY PLOT

The discrepancy plot illustrates the difference between the observed ECR and that which would apply to an ideal instrument, that is, one that has no curvature in the ECR. In the ideal case, the ECR would be a linear equation, such as,

$$E(c) = Z + s \cdot c$$

where E is energy in keV, Z is the detector zero off-set, s is the slope, and c represents the spectrum channel axis. This equation is fitted to the refline data using the associated uncertainties as weights.

The discrepancy of each peak, d_j , is determined using the following equation:

$$d_j = E_j - s \cdot c_j$$

where d_j is the discrepancy value for peak j , E_j is the known energy for the photon represented by peak j , s is the slope of the first-order weighted simple linear regression, and c_j is the centroid channel for peak j . If an instrument were perfectly linear and had zero offset, $d_j = 0$.

As shown in [Figure 12](#), error bars accompany the discrepancy values as well as the ECR (green) adjusted to the plot scale. The equation for the adjusted ECR, $\Delta(c)$, is as follows:

$$\Delta(c) = \xi_0 + (\xi_1 - s)c + \xi_2 c^2 + \xi_3 c^3$$

The discrepancy plot illustrates how well the ECR matches the observed data.

Resolution Function Plot

The detector resolution plot is simply a graph of the refline locations (in energy) and their resolutions as estimated from the peak fit routine. The RER calibration equation is also included in the plot. The form of the RER can be found in “RER Update” on page 26. An example of a resolution function plot is located in [IDC6.5.10Rev1].

Efficiency Function Plot

This graph includes the efficiency pair data as well as a plot of the EER equation. The pair data is from the last detector calibration. The form of the EER is in “Efficiency Conversion” on page 28. An example of an efficiency function plot is located in [IDC6.5.10Rev1].

Region of Interest Dialog Window

In this window ([Figure 13](#)), users with the correct permissions can insert, remove, and modify the peaks found during automatic analysis. After peak modification, a peak fitting algorithm (described in [Eva99b]) is run, Canberra’s NID function is rerun, and the results are displayed. The analyst can accept the changes or modify the peaks again. A

▼ Interactive Analysis

differences window is available for displaying the resulting changes. When the analyst has finished modifications, the results are saved to the database or cancelled. The changes reported in the differences window are reported in the RRR.

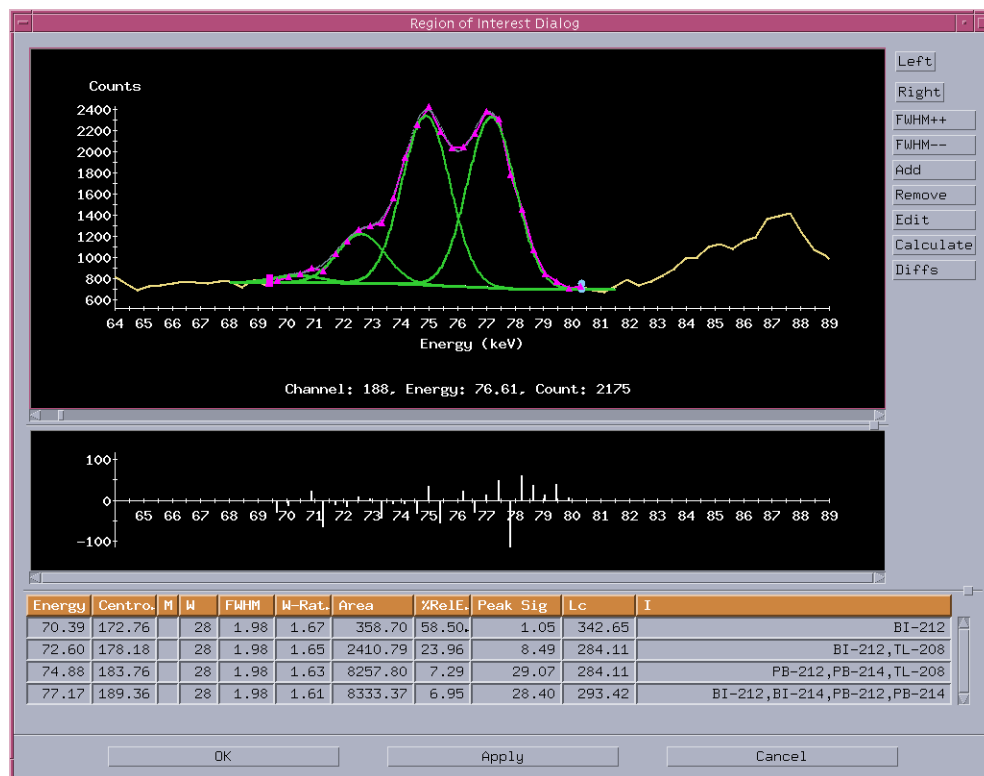


FIGURE 13.INSPECTRA REGION OF INTEREST DIALOG WINDOW

Multiplet ROI

Users can now insert, remove, and modify peaks occurring within the same ROI (that is, multiplets).

W-Ratio

The W-Ratio is the ratio of 'W' to 'FWHM'. W is the actual peak FWHM where 'FWHM' is the FWHM of the peak predicted by the RER.

Peak Significance

This parameter also shows up in the Peak Search Dialog window and is calculated using the following equation.

$$\text{PeakSig} = \frac{\text{Area}}{L_c}$$

where Area is the peak net area and L_c is the critical limit [Bie00a].

Compare Dialog Window

The compare dialog allows one to compare the current sample spectrum to others. Available comparators include the MRP sample spectrum, the MRP blank spectrum for that detector, the PREL spectrum for that sample, and any other sample spectrum one may choose. For FULL sample spectra, another comparator is the "closest" sample spectrum. This spectrum is a FULL sample from the same detector and station that most closely matches the current sample for the following criteria:

- Collection time
- Decay time
- Acquisition time
- Blower flow rate
- ^{212}Pb concentration

The "closest" sample spectrum has the minimum Euclidean distance between its parameters (given above) and those of the current sample.

Nuclide Review Window

The nuclide review screen displays multiple regions in a spectrum where photon lines for a chosen nuclide would be observed. The regions for the four photons of highest abundance are available for display. Each region is ordered on the screen according to the photon abundance from highest to lowest. An example of this window can be found in [IDC6.5.10Rev1].

An option available in this window is the “Pseudo” peak function. When this option is checked, pseudo-peaks appear in each region. These peaks show what each photon line would look like at a concentration equivalent to the MDC for that nuclide.

The pseudo-peaks are Gaussian (see Figure 7 on page 23) and the equations that describe each are determined by first finding the required net peak area, S , to correspond to the MDC values (located in **gards_nucl_ided**), that is,

$$S = \left(\frac{C\epsilon y F \vartheta}{\lambda^2} \right) (1 - e^{-\lambda t_s})(e^{-\lambda t_p})(1 - e^{-\lambda t_r})$$

where C is the MDC in $\mu\text{Bq}/\text{m}^3$, F is the average blower flow rate in m^3/hr , ϵ is the detector efficiency in counts per emitted photon, y is the photon abundance (or intensity) in photons per decay, ϑ is a factor used for unit conversions, t_s is the sample collection duration in seconds, t_p is the time between the collect stop and the acquisition start, t_r is the acquisition duration in clock time (vs. live time), and λ is the decay constant in s^{-1} . This equation is derived using concepts presented in “Nuclide ID and Quantification” on page 29 and by assuming that the acquisition live time is approximately equal to the acquisition real time, or clock time. The peak centroid channel, c_p , is determined from the expected line energy in **gards_nucl_lib** as well as the ECRU relation (see “ECRU Update” on page 25). The peak width metric, σ , is determined from the expected line energy, the RERU relation (see “RERU Update” on page 26), and the equation below:

$$\sigma = 2.355 \cdot \text{FWHM}$$

The peak height is calculated according to

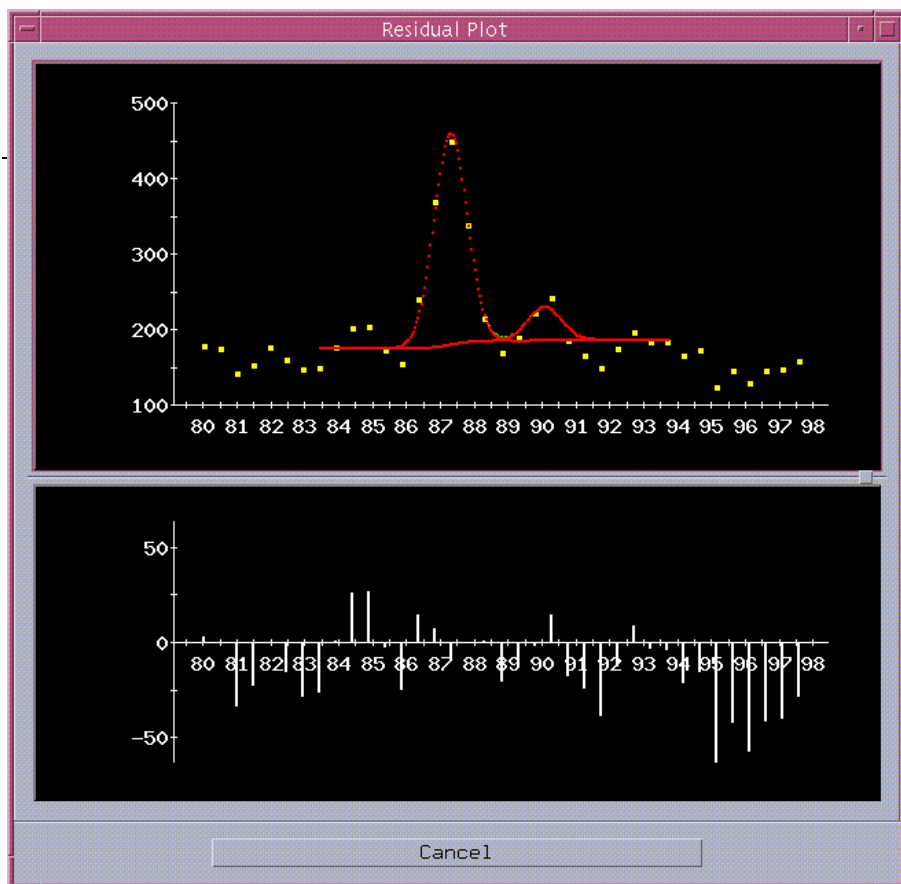
$$H = \frac{S}{\sigma \sqrt{2\pi}}$$

The pseudo-peak adjuster in the Inspectra Nuclide Review window is used to scale the nuclide concentrations to values higher than the MDC in integer multiples. The pseudo-peaks automatically adjust themselves after each scaling.

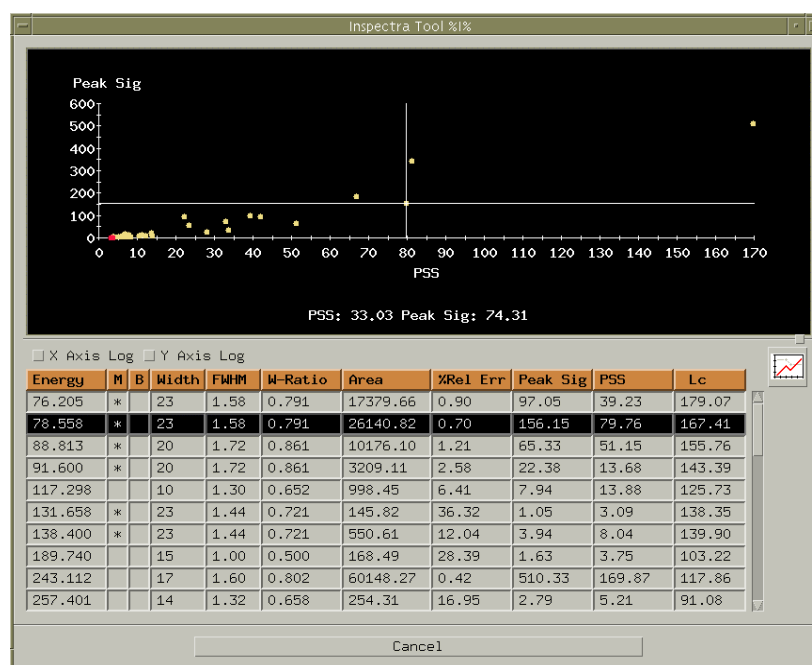
Residual Plot Window

The residual plot is a line graph of the difference between the actual counts in a peak channel and the peak fit at that channel. This number can be either positive or negative and illustrates how well a peak fit matches the observed counts. Included on top of the residual plot is the ROI of interest with the peak fit (red). An example of a residual plot window is below ([Figure 14](#)).

▼ Interactive Analysis

**FIGURE 14.INSPECTRA RESIDUAL PLOT****Peak Search Sensitivity vs. Peak
Significance Scatter Plot**

A scatter plot displaying the Canberra Peak Search Sensitivity (PSS) vs. the peak significance for each peak is available in Inspectra. (See Figure 15.) This plot can help an analyst determine if a peak is real.



**FIGURE 15. PEAK SEARCH SENSITIVITY VS. PEAK SIGNIFICANCE
SCATTER PLOT IN INSPECTRA**

As mentioned in “Peak Locate” on page 19, the Canberra peak locate algorithm uses the Generalized Second Difference Method to find peaks in a spectrum. As part of this algorithm, the peak search sensitivity (PSS) is determined for each peak. Please refer to [Can97] for details on the calculation of this parameter. The peak significance is calculated according to the following formula

$$\text{PeakSig} = \frac{\text{NetArea}}{L_c}$$

and is a metric of how the peak area compares to the critical limit, L_c . Guidance for determining if a peak is real can be obtained by observing where the PSS and peak significance fall on the plot as shown in Figure 16.

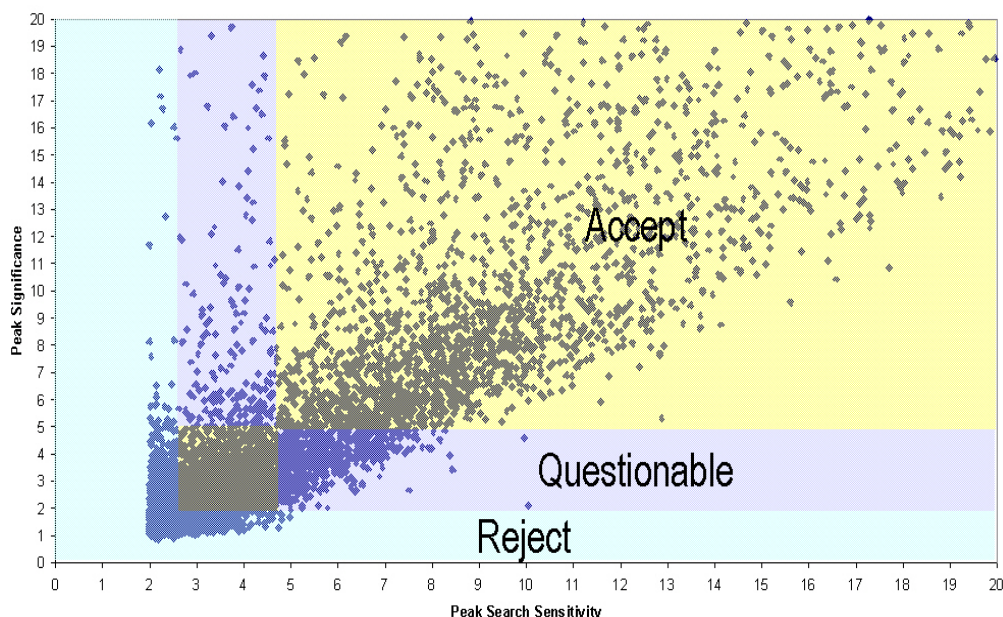


FIGURE 16. TWO DIMENSIONAL PEAK DETERMINATION APPROACH

This window also displays a table which contains the peak list and has the following columns: Energy, M (multiplet flag), B (background flag), Width (peak width in channels), FWHM (full width at half maximum), W-Ratio (FWHM ratio), Area, %Rel Err (percent relative uncertainty of peak area), Peak Significance, PSS, and L_c . By clicking on a peak in the peak list, the graph cross-hairs hone in on the associated plot point.

Peak Search Dialog Window

A feature of the Peak Search Dialog window is the nuclide line activity. When this option is checked after highlighting a nuclide line in the Peak Search window, a Nuclide Line Activity window is created. This window lists the photon energies in the nuclide library associated with the decay of the nuclide of interest, along with photon abundances, actual peak areas, and predicted peak areas. For the photon line of highest abun-

dance, the predicted area is assigned to be 100(%). The predicted areas for the remaining photon lines, PA_i , are given as a percentage of the predicted area of the photon line of highest abundance. The calculation is as follows:

$$PA_i = PA_h \cdot \left(\frac{I_i}{I_h} \right) \cdot \left(\frac{\epsilon_i}{\epsilon_h} \right)$$

where $PA_h = 100$ is the predicted area of the peak of highest abundance, I is the photon abundance, and ϵ is the detector efficiency from the EER for that photon energy.

Categorization Dialog Window

The category is the current priority level of the sample. This value may change upon analyst editing of the automatic analysis results. The same algorithm used in “Prioritization” on page 56 is used to assign the category level. The category upon release is the level retained for the sample.

The parameters ‘lower limit’ and ‘upper limit’ are from the EWMA or RDC calculations during the prioritization determination. See “Prioritization” on page 56 for more details.

MDC Dialog Window

In the MDC Dialog window, the values in the ‘Min MDC’ and ‘Max MDC’ columns are obtained from **gards_mdas2report** table. These values are entered directly into the database table by a user with the correct permissions and are not used in any data processing.

Sample Source Dialog Window

The information in the top half of the Sample Source Dialog window is obtained from **gards_stations**. The information in the bottom half is from **gards_detectors**.

Sample Detail Dialog Window

Included in the Sample Detail Dialog window are average values for the sample quantity (m^3), the blower flow rate (m^3/hr), sampling time, decay time, and acquisition time. A standard deviation for the quantity is also given. These numbers are calculated for a particular station for the most recent 30 days. An example of the Sample Detail Dialog window can be found in [\[IDC6.5.10\]](#).

Other information displayed in this window is obtained from **gards_sample_data** and **gards_sample_status**.

CORIAN T

Depending on the roles assigned to a user, this software tool allows one to view sample data acquired from detectors employing 3-D beta-gamma coincidence detection, view other sample data, and add comments to a sample. This section discusses the scientific premises used in the CORIAN T software tool.

Histogram Plot

The colors assigned to each point are determined from the number of counts in the β - γ coincidence channel. Colors are assigned according to the table below.

TABLE 5: HISTOGRAM PLOT COLORS

Counts	Color Name	Color Values (Red, Green, Blue)
0	dark blue	0, 0, 150
1	cyan	0, 255, 255
2	green	0, 255, 0
3	yellow	255, 255, 0
4	pink	255, 175, 175
30	red	255, 0, 0
256	white	255, 255, 255

If a count value falls between two colors, the color values are linearly interpolated to adjust the color.

Isotope Tab Windows

Below are the scientific principles behind the features in the five isotope tabs: PB-214, XE-135, XE-133, XE-131M, and XE-133M.

Beta-Gated Gamma Spectrum

This plot is the β -gated gamma spectrum calculated for the ROI, and hence, nuclide of interest. Each point on the graph corresponds to the sum of the counts in each row of the 2-D ROI.

Gamma-Gated Beta Spectrum

This plot is the γ -gated beta spectrum calculated for the ROI, and hence nuclide, of interest. Each point on the graph corresponds to the sum of the counts in each column of the 2-D ROI.

Pie Chart

The pie charts in each isotope tab window graphically display the percentage for each contribution (net Compton continuum background, gas cell background, detector background, and interference from other nuclides) to the gross counts. Negative counts are not displayed.

Beta Graph

The Beta Graph is the result of summing all the columns in the Histogram. Highlighted areas from left to right are ROIs 5 and 6, corresponding to the areas where the conversion electron signals of ^{131m}Xe and ^{133m}Xe , respectively, are expected. See Figure 17.

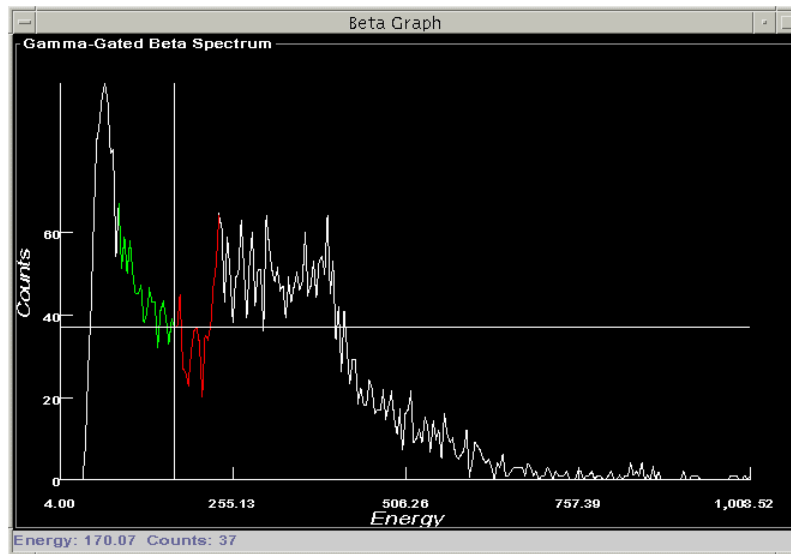


FIGURE 17. CORIANT BETA GRAPH

Gamma Graph

The Gamma Graph is the result of summing each row in the Histogram. Highlighted areas from left to right are ROIs 4, 3, 2, and 1, corresponding to the areas where the following radionuclide signals are expected:

- $^{131\text{m}}\text{Xe}$, ^{133}Xe , $^{133\text{m}}\text{Xe}$ - ROI 4
- ^{133}Xe with possible ^{214}Pb interference - ROI 3
- ^{135}Xe with possible ^{214}Pb interference - ROI 2
- ^{214}Pb - ROI 1

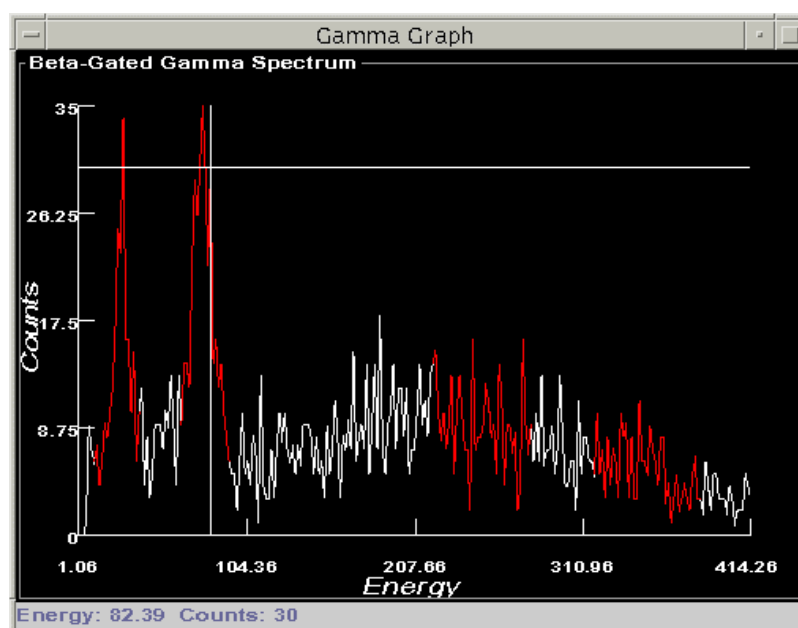


FIGURE 18. CORIANT GAMMA GRAPH

TRENDVUE

The purpose of Trendvue is to visualize historical PHD and state of health data. This functionality enables analysts to discriminate trends or observe unusual occurrences. The tool is not equipped to perform any data analysis. For more information on Trendvue, see [IDC7.1.10Rev1] and [IDC6.5.10Rev1].

ANALYST WORK AREA

The purpose of the Analyst Work Area is to provide a system status/health overview of all stations sending radionuclide information to the IDC. The tool is not equipped to perform any data analysis. For more information on the Analyst Work Area tool, see [IDC7.1.10Rev1] and [IDC6.5.10Rev1].

RMS WORKFLOW

The purpose of RMS Workflow is to visually display the receipt of data at the IDC as well as the state of blowers and detectors at stations and laboratories, with respect to time. This tool is not equipped to perform any data analysis. For more information on RMS Workflow, see [IDC7.1.10Rev1] and [IDC6.5.10Rev1].

DATA WORKBENCH

The purpose of Data Workbench is to provide a direct interaction with the RMS database and allow maintenance of the reflines associated with a station/detector combination. The tool is not equipped to perform any data analysis. For more information about the Data Workbench tool, see [IDC7.1.10Rev1] and [IDC6.5.10Rev1].

PROCESSING TOOLS

The RMS Processing Tools allows many software units associated with automatic and post-analysis processing to be performed manually. This functionality is necessary for spectra that fail during these processing steps. The software units available in the Processing Tools package are:

rms_acd
rms_analyze
rms_categorize
rms_DB_flags
rms_db_to_cnf
rms_db_to_nlb
rms_mar_auto
rms_nlb_to_db
rms_pairs
rms_phd_report
rms_rrr_report, *rms_ssreb_report*, *rms_rnps_report*, *rms_xe_rrr_report*
rms_xanalyze

See Chapter 9, “Processing Tools” in [IDC6.5.10Rev1] for descriptions of these software units. Out of all the software units in RMS Processing Tools, only *rms_analyze*, *rms_xanalyze*, and *rms_categorize* have analytical capabilities. The scientific principles behind these calculations are the same as those described in Chapter 2.

▼ Interactive Analysis

Chapter 4: Post-analysis Processing

| This chapter describes immediate and delayed post-analysis IDC processing and includes the following sections:

- Overview
- Creating Final Data Products

RRR and SSREB. These data products are available by request or subscription (see [IDC3.4.1Rev2]), or can be obtained from the Radionuclide Web page (see [IDC7.1.10Rev1]).

Included in the RRR is the Field of Regard (FOR) for that sample. The FOR is an area within which air has a non-zero probability of moving over a station during a specific time interval, and is included in the RRR as a .gif image. FORs are determined automatically each day for every operating radionuclide station and are saved to the directory `~/FOR/station_code/year/day`. The time interval represented by each FOR is 24 hours, beginning at 00:00 UTC and ending at 23:59 UTC.

The collection start and stop times for a sample may not coincide with the FOR start and end times. In addition, a sample may have been collected for longer than 1 day. To determine which FOR to include in the RRR, the total sampling duration is determined using the sample *collect_start* and *collect_stop* times. The date on which the mid-point of the sampling duration occurs, as well as the *station_code*, are used to retrieve the appropriate FOR from its directory to include in the data products.

If a sample has a corresponding RLR when an SSREB is created, the #Header and #Conclusion sections of the RLR will be automatically included in the Certified Laboratory Results section of the SSREB. Additions can be made to the SSREB via the SSREB Revision Tool when new event data is received and processed. An example of an SSREB can be found in [IDC3.4.1r3].

The analysis results of the past three days are summarized daily in the RNPS. This data product is created by a CRON job triggered every 24 hours. An example of an RNPS can be found in [IDC3.4.1r3].

▼ Post-analysis Processing

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Glossary

Symbols

2-D

Two-dimensional.

3-D

Three-dimensional.

β

Beta, as in beta particle.

γ

Gamma, as in gamma ray.

μBq

MicroBecquerels.

A

abundance

Fraction of a decay event that results in the radiation(s) of interest (for example, a γ line at a specific energy or a β - γ coincidence pair). Intensity is used synonymously with abundance.

acquisition live time

Time multichannel analyzer (MCA) electronics is available for processing pulse amplitude signals; equivalent to acquisition real-time less detector dead-time, reported in seconds.

acquisition real time

Total elapsed clock time a sample is counted, reported in seconds.

acquisition start

Time at which the detection system at a station commences sample acquisition.

acquisition stop

Time at which the detection system at a station completes sample acquisition.

activation products

Nuclides produced from the absorption of neutrons by a nucleus.

activity

Decay rate of a radionuclide; this quantity is usually expressed in Becquerels (disintegrations per second), Bq.

ALERT

Alert message. Data type that includes ALERT_FLOW, ALERT_SYS, ALERT_TEMP, and ALERT_UPS.

anthropogenic

Man-made, not of natural origin.

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APE

Average Prediction Error.

ARR

Automatic Radionuclide Report. This report is a product of the automatic data processing and includes sections describing the sample information, prioritization results (noble gas only), sample activity, MDCs for key nuclides, peak search results and notes, processing parameters, update parameters, data quality flags, event screening flags, calibration equations, and field of regard.

B**background**

Contribution to a spectrum from naturally occurring radionuclides as well as interactions between radiation and materials in the vicinity of the detector.

baseline

Contribution to a spectrum from the partial energy deposition of a γ -ray or gamma ray in a detector.

Becquerel

Unit of activity equal to one disintegration per second.

beta-gamma coincidence efficiency

Ratio of counts detected in a 2-D ROI to the actual amount of photons emitted by a sample in coincidence with an electron; depends on detector configuration, geometry, and ROI boundary limits.

beta-gamma coincidence event

Nuclear decay that produces both a γ -ray and a β particle within a very short time scale; may also refer to other photon-electron coincidence events such as an X-ray with a conversion electron.

beta-gated gamma spectrum

A γ spectrum in which all photons counted were detected in coincidence with an electron.

beta particle

Electron that is produced from a nuclear decay. May also refer to other electron radiations, for example, a conversion electron.

BLANKPHD

Blank Pulse Height Data; ASCII data message transmitted to the IDC that contains the pulse height data of an unexposed air filter as well as other information in an IDC-approved format.

Bq

Becquerel.

C**CALIBPHD**

Calibration Pulse Height Data; ASCII data message transmitted to the IDC containing the pulse height data of a certified standard source as well as other information in an IDC-approved format. The data in a CALIBPHD is used to determine the ECR, EER, and RER.

category

Number from 1 to 5 assigned to a radionuclide sample during interactive analysis indicating the presence of certain types of nuclides. Category 1 indicates a spectrum with normal natural nuclides while 5 indicates spectra with multiple anthropogenic nuclides.

centroid

Energy (in keV) or channel number at the center of a photopeak.

centroid channel

Spectrum channel at the center of a photopeak.

channel

An energy window (in keV) representing a differential increment of pulse height.

CIX

Confidence Index.

CLT

Critical Level Test.

cm

Centimeter.

.cnf

Canberra Nuclear Format.

collection start

Time at which the collection equipment at a station commences sample collection.

collection stop

Time at which the collection equipment at a station completes sample collection.

comments

Free text field containing comments made by a station operator or IDC analyst.

conversion electron

Electron emitted from an atomic electron shell, usually in coincidence with an X-ray.

CORIAN

Coincident Radiation Interactive Analysis Tool.

cosmic nuclide

Nuclides produced by the interaction of cosmic-rays with matter.

cosmic ray

General term for radiation originating from the cosmos. Includes primarily protons and alpha particles, but may also include electrons and nuclei of atomic number between 4 and 26.

cosmogenic nuclide

See cosmic nuclide.

COTS

Commercial, Off-the Shelf.

critical level

Minimum net counts that must be contained in an ROI for reliable nuclide detection (L_c).

CTBT

Comprehensive Nuclear Test-Ban Treaty.

D

data type

Kind of data in a data message; possible data types include ALERT_FLOW, ALERT_SYS, ALERT_TEMP, ALERT_UPS, ARR, BLANKPHD, CAL-IBPHD, DETBKPHD, GASBKPHD, MET, QCPHD, RLR, RMSSOH, RNPS, RRR, SAMPLEPHD, and SSREB.

decay time

Time duration an exposed filter is allowed to decay before data acquisition.

DETBKPHD

Detector Background Pulse Height Data; ASCII data message transmitted to the IDC containing the pulse height data from a background count as well as other information in an IDC-approved format.

E

ECR

Energy (vs.) Channel Regression; an equation providing the detector-specific relationship between channel number and energy.

ECRU

Energy (vs.) Channel Regression Update; an equation providing the updated detector-specific relationship between channel number and energy.

EER

Energy (vs.) Efficiency Regression; an equation providing the detector-specific relationship between efficiency and energy.

efficiency

Ratio of counts detected under a photopeak to the amount of radiation quanta emitted by a sample; depends on detector configuration and geometry. This parameter is unitless.

energy

Usually refers to the measured kinetic energy of radiation quanta deposited in a detector. the unit most appropriate for such measurements is keV.

energy span

The energy interval over which a multi-channel analyzer counts radiation quanta. Usually equivalent to the highest energy on the γ or β axis, rounded to the nearest 100 keV.

event

Occurrence that displays characteristics indicative of a possible nuclear weapons test.

EWMA

Exponentially Weighted Moving Average.

F

field of regard

An area within which air has a non-zero probability of moving forward with atmospheric flow over a specific time interval to arrive at a station, and is included in the ARR and RRR.

FIR

Finite Impulse Response; a digital filtering technique.

fission products

Nuclides produced from fission.

flow rate

Air volume passing through a blower per unit time; reported in scm (m³)/hr.

FOR

Field of Regard.

FULL

Full; spectral identifier indicating that the sample has been counted for the total acquisition duration.

FWHM

Full Width at Half-Maximum; metric of detector resolution and equivalent to the width of a photopeak (in keV) taken at the peak height equal to half the maximum peak counts.

G**gain**

Amplification of the measured energy deposition in a radiation detector. This is achieved through the use of electronic amplifiers.

gamma

Gamma-ray.

gamma-gated beta spectrum

β spectrum in which all electrons counted are detected in coincidence with a photon.

gamma ray

Photon that is produced from a nuclear transition. May also imply other photon radiations, for example, an X-ray.

GASBKPHD

Gas Background Pulse Height Data. Data type sent by noble gas monitoring systems that observe a memory effect during sample acquisition. This effect is due to atoms from the previous sample adsorbed onto the walls of the gas cell. The counts from the memory effect must be subtracted from the sample counts for accurate activity quantification.

H**half-life**

The time required for a radionuclide to decay to half its initial activity.

histogram

Two-dimensional array containing β - γ coincidence counts. One axis represents γ channels (or energy) while another represents β channels (or energy). The data in a histogram may be plotted in 3-D or as a 2-D contour plot.

HPGe

High-Purity Germanium Detector.

hr

Hour(s).

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I**IDC**

International Data Centre.

IMS

International Monitoring System.

K**keV**

Kiloelectron Volts; a metric of radiation kinetic energy.

keyline

The γ -ray of a radionuclide with the highest detection probability and no interference, for a specific nuclide.

L **L_c**

Critical Level [Cur68].

 L_D

Detection Limit [Cur68].

M**m**

1. Meters.
2. SI prefix meaning milli-.

mBq

milliBequerel.

MDA

Minimum Detectable Activity.

MDC

Minimum Detectable Concentration.

mean-squared error

An estimate of the average variance of a parameter.

MET

Meteorological message; one of the many radionuclide data types.

minimum detectable concentration

Activity concentration of a given radionuclide below which signals are indistinguishable from the measurement process noise level.

MRP

Most Recent Prior; the sample counted most recently on the same detector and originating from the same station as the sample presently being analyzed.

MSE

Mean-squared error.

multiplet

A spectrum region of interest composed of more than one photopeak.

N**natural radioactivity**

Radioactivity from cosmogenic and primordial nuclides that is always present on earth.

net area

Equal to the integrated photopeak counts minus the baseline and background counts, interference counts, and memory effects.

NID

Nuclide Identification.

NL

Nuclide Library.

noble gas

A noble element of the periodic table: He, Ne, Ar, Kr, Xe, and Rn.

nuclide

One of many combinations of nucleons that may comprise an atomic nucleus. Because all nuclides of interest with respect to CTBT compliance verification are radioactive, this term is often used to refer specifically to radionuclides.

O**ODE**

Ordinary Differential Equation.

P**PE**

Prediction Error.

peak

A statistically significant increase in counts above a spectrum baseline at an energy associated with a gamma line of a particular radionuclide or other phenomenon.

PHD

Pulse Height Data; a format for spectral data messages transmitted to the IDC. Possible PHD data message types include SAMPLEPHD, GASBKPHD, BLANKPHD, DETBKPHD, CALIBPHD, and QCPHD.

PIDC

Prototype International Data Centre.

PIF

Prediction Interval Filter.

PLSQL

Programming language for the database.

PREL

Preliminary; usually referring to a SAMPLEPHD with an acquisition time less than that of the full acquisition duration.

priority

1. Number from 1 to 4 automatically assigned to an identified nuclide indicating whether or not the nuclide is natural or anthropogenic and if the nuclide is above or below normal observation levels.
2. Number from 1 to 5 assigned to a radionuclide sample during automatic analysis indicating the presence of certain types of nuclides. Category 1 indicates a spectrum with normal natural nuclides while 5 indicates spectra with multiple man-made nuclides.

progeny

A radionuclide that comes into being due to the decay of a parent.

Q

QCPHD

Quality Control Pulse Height Data; ASCII data message transmitted to the IDC containing the pulse height data of a certified standard source as well as other information. The QCPHD, along with other information, is used to check a detector's state of health.

quantity

Collected air volume in scm; same as sampled air volume.

R

radioactivity

See activity.

radionuclide

A nuclide that has an unstable nucleus, that is, a radioactive nuclide.

radionuclide laboratory

These are laboratories listed in Annex 1 of the CTBT and include any laboratories that are certified by the IMS/IDC in the future.

refline

Photon lines of high intensity typically generated by natural nuclides.

region of interest

Region of a radionuclide spectrum or histogram that corresponds to a particular radionuclide.

RER

Resolution (vs.) Energy Regression; an equation providing the updated detector-specific relationship between resolution and energy.

RERU

Resolution (vs.) Energy Regression Update; provides the updated detector-specific relationship between resolution and energy.

resolution

Metric of a detector's ability to detect photons at discrete energies and is equivalent to the FWHM; see FWHM.

RLR

Radionuclide Lab Report; report containing sample analysis results from a certified radionuclide laboratory.

RMS

Radionuclide Monitoring System; the part of the IMS that monitors the atmosphere for radionuclides originating from a nuclear weapons test.

RMSSOH

Radionuclide Monitoring System State of Health message; one of the many radionuclide data types.

RNPS

Radionuclide Network Product Summary; daily report containing a compilation of the status of collection, processing, and analysis of particulate and noble gas data for a 3-day period.

ROI

Region of Interest.

ROI number

Integer from 1 to 6 assigned to a 2-D ROI for the analysis of 3-D β - γ coincidence data.

RRR

Reviewed Radionuclide Report. Electronic file containing the results of the interactive review of the automated radionuclide processing. It contains sections on sample information, measurement categorization, measured radionuclide quantities, MDCs, radionuclide identification, analyst editing, processing parameters, data quality flags, event screening flags, calibration equations, and field of regard.

S**s**

Second(s).

sample

The solid or gaseous entity collected by a blower at an RMS station that is analyzed for its radioactive contents.

sample ID

Unique identification number assigned to a sample by the IDC.

SAMPLEPHD

Sample Pulse Height Data; ASCII data message containing pulse height data acquired by counting a gas or particulate sample with a detector system.

scm

Standard cubic meter(s).

singlet

Spectrum photopeak consisting of counts from one mono-energetic γ -ray; photopeak containing counts from multiple gamma-rays, but fit as if it is comprised of counts from only one because contributions from the individual radiations cannot be separated, as in a multiplet.

SOH

State-of-health.

spectrum

A plot of the differential number of pulses (in counts) per differential pulse height (in channels or keV).

SPHD

Sample Pulse Height Data; ASCII data message containing the pulse height data of a sample, as well as other information. The two types of SPHDs are full (FULL) and preliminary (PREL).

SQL

Structured Query Language.

SSREB

Standard Screened Radionuclide Event Bulletin; bulletin generated by the IDC when fission or activation products are detected at a radionuclide station above normal limits. A SSREB contains information on the possible event, source location, fission products, activation products detected, any isotopic ratios calculated, and any certified laboratory results. New event

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information can be added to the SSREB as it arrives, therefore, multiple revisions of an SSREB are possible.

standard cubic meter

Volume occupied by 1 m³ of gas at 0 C and 1013 hPa.

SVD

Singular Value Decomposition.

T**Type I error**

Spectral region of interest falsely identified as a peak by the automated processing.

Type II error

Peak undetected by the automated processing.

U**uncertainty**

Estimate of the deviation from the true mean for a parameter or variable of interest.

UTC

Universal Time Coordinate.

W**WWW**

World Wide Web. The portion of the Internet that allows the display of formatted pages of text and graphics.